TECHNICAL ASSISTANCE DOCUMENT:

GUIDELINES FOR THE PETITIONER AND REVIEWER

ON THE COMPUTER SIMULATION OF HAZARDOUS WASTE INJECTION

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INTRODUCTION

Amendments to the Resource Conservation and Recovery Act (RCRA) enacted through the Hazardous and Solid Waste Amendments of 1984 (HSWA) prohibit the continued land disposal of untreated hazardous wastes beyond specified dates. The legislation specifically defines land disposal to include, but not be limited to, any placement of hazardous waste in a landfill, surface impoundment, waste pile, injection well, land treatment facility, salt dome, salt bed formation, or underground mine or cave. In particular, the legislation requires that the United States Environmental Protection Agency (EPA) must determine if the injection of hazardous wastes poses any threat to health or environment. The disposal by injection of solvents, dioxins, and California list wastes are specifically prohibited in Section 3004(f) of RCRA if it may be "reasonably determined that such disposal may not be protective of human health and the environment for as long as the waste remains hazardous." These, and other listed wastes, which are prohibited from injection, may be injected under two circumstances:

1) when the waste has been treated in accordance with the requirements of 40 CFR Part 268 pursuant to Section 3004(m) of RCRA, or
2) when the applicant has demonstrated that there will be no migration of hazardous constituents from the injection zone for as long as the waste remains hazardous.

Since both RCRA Section 3004 (f) and (g) require a demonstration that injection is protective of human health and the environment, the Agency believes that the no-migration standard should apply to all Class I hazardous waste injection wells, regardless of the type of injected waste. For this reason, EPA has proposed the use of a petition process and standard that is the same for all banned hazardous wastes that are injected whether they fall under Section (f) or (g).

According to the regulations, applicants who do not qualify for exemption from the ban under (1) above must demonstrate that there will be no migration of hazardous constituents from the injection zone for as long as the waste remains hazardous. This "no-migration" requirement for injection wells can be satisfied in either of two ways.

1) The applicant could demonstrate that waste constituents would not migrate from the injection zone in hazardous concentrations. EPA has proposed that applicants must show that before any injected fluids leave the injection zone, the wastes would not be considered hazardous and would not contain hazardous constituents which would result in a threat to human health or the environment. The Agency will only grant an exemption if the applicant shows that any hazardous constituents would not leave the injection zone in concentrations higher than EPA-recommended health-based limits. At the present time these include Maximum Contaminant Levels (MCLS), (promulgated pursuant to the Safe Drinking Water Act), water quality standards and criteria

(Ambient Water Quality Criteria 45 FR 79318, November 28, 1980; 49 FR 5831, February 15, 1984; 50 FR 30784, July 29, 1985), health-based limits based on verified reference doses developed by EPA's Risk Assessment Forum (Verified Reference Doses of USEPA, ECAO-CIN-475, January 1986) and Carcinogenic Potency Factors (CPF) developed by EPA's Carcinogenic Assessment Group to be used to determine exposure at a given risk (Table 9-11, Health Assessment Document for Tetrachloroethylene (Perchlorethylene) USEPA, OHEA/600/8-82/005F, July 1985) or site-specific EPA-approved public health advisories issued by the Agency for the Toxic Substance and Disease Registry of the Center for Disease Control, Department of Health and Human Services.

EPA is currently compiling toxicity information on many of the hazardous constituents contained in Appendix VIII to Part 261. However, for some hazardous constituents, EPA recommended exposure limits do not yet exist. In these situations, EPA is proposing that an applicant show that the concentration of the constituent would not exceed a level three orders of magnitude below detection levels at the edge of the injection zone. In addition, an applicant would also need to demonstrate that wastes, deemed hazardous due to the characteristic of Extraction Procedure (EP) toxicity, would not migrate beyond the injection zone at concentrations above EPA-recommended limits. Also, an applicant would be required to show that wastes deemed hazardous due to characteristics of ignitability, corrosivity, or reactivity would not display these characteristics beyond the injection zone.

According to the proposed regulations, the no-migration petition could be satisfied by demonstrating that the constituents would be transformed to non-hazardous by-products, or that concentrations would be reduced to non-hazardous levels within the injection zone itself. For the purposes of this demonstration, the applicant is not required to account for constituents which were present in the formation fluid prior to injection.

2) Alternatively, the applicant could attempt to demonstrate, using flow and transport models, that the site conditions are such that injected fluids would not migrate vertically upward out of the injection zone, or migrate within the injection zone to a point of discharge, over a time span of 10,000 years. Demonstrations of this type are expected to be easier to perform and review than those under paragraph (1). The principles of fluid flow in deep formations are well understood, when compared to the state of knowledge of waste transformations. Use of flow and transport simulators developed by the petroleum industry or the U.S. Government would be appropriate in these demonstrations.

EPA has recognized that in some areas, a natural pressure gradient may exist which would result in movement of injected fluids after closure of the injection well(s). There is a need, therefore, to provide post-injection analysis for some period of time. The 10,000 year period was selected for two reasons. First, EPA believes that formations which contain injected fluids for this period will in all

probability, contain the fluids over a much longer period. Secondly, evidence exists which suggests that the long residence time of the waste in the injection zone will give a reasonable degree of certainty that the waste will no longer be hazardous.

EPA anticipates that most applicants will first try to satisfy the regulatory requirements under the 10,000 year containment provision in paragraph (2). The applicants would determine the area over which the waste front would travel during a 10,000 year period using fluid flow simulators. If the simulation indicated that some wastes would leave the injection zone, it may be possible by analysis of waste transformation, immobilization or other physical processes to show that no restricted constituents would leave the zone in hazardous concentrations. Alternatively, applicants may choose to show that the wastes will transform to non-hazardous concentrations or non-restricted constituents in a timespan of less than 10,000 years. In this way, the length of time required for containment would be reduced.

Due to the nature of hazardous waste injection, it is usually not possible to directly confirm whether migration out of the injection zone is occurring, or will occur in the future. The proper location of monitoring wells that can effectively detect waste migration is difficult, and in addition, these wells can be expensive to drill. For this reason, applicants and reviewers will have to rely heavily on the results of the mathematical simulations in determining the safety of each proposed injection site. Due to this reliance on simulation

results in the approval process it is extremely important that the simulations be performed and reviewed correctly. It is the purpose of this manual to outline the proper procedures required to correctly simulate the injection of hazardous wastes. This manual is directed towards the EPA and/or State Agency reviewer but will be useful to the applicant as well.

This manual has been designed as a practical guide to the simulation injection of hazardous waste. For this reason, most of the theory and mathematics on which modern simulators are based have been omitted from the text. The Appendices contain further discussion of Analytical Well Test solutions and superposition. This information may be of interest to some readers.

The first section (of this manual), **Nature of Mathematical Simulators,** provides a brief overview of the concepts involved in most numerical simulators of fluid flow in porous media. These concepts provide a fundamental understanding of the principles upon which these simulators are based. The perspective provided by this understanding can assist in making the proper decisions when performing or evaluating a simulation study. For those already familiar with these principles, this section can be skipped. However, it is expected that many of the users of this manual will be unfamiliar with the technology of numerical simulation. For these users simulators will remain essentially a "black box" even after a review of this section. With some care, however, these users can satisfactorily perform or evaluate

a simulation study. The purpose of this manual is to provide some "road signs" as to when one should "stop, look, or listen" or "proceed with caution." We will describe herein what a proper data set is comprised of, and how to judge proper simulation performance. For those readers who wish more exposure to numerical simulation fundamentals the literature contains several excellent references: Thomas(1982), Peaceman(1977), Aziz and Settari(1979), and Crichlow(1977) contain material describing numerical simulation.

The subsequent sections of this manual offer a practical guide to the performance of a simulation study of hazardous waste injection. These sections are presented in the same order as an engineer or geologist might perform the steps of such a study. The first step is to understand and define the problem. The **Problem Types/Simulator Selection** section of this report discusses the different combinations of geology and fluids often encountered in waste injection. This section illustrates how to identify each type of problem and which parameters will be the primary controls of fluid flow for each type. After identifying the problem type, an appropriate simulator can be selected. This section discusses the various types of simulators available today. It discusses which simulators are suited for which types of problems. This section will assist the user in avoiding overkill or underkill. That is, it will guide the engineer in selecting a simulator which is of the proper technical level for the complexity of the problem. It will help to avoid selecting a simulator which does not accurately model the problem, or which provides either too little or too much

detail in the results. It should be noted that specific brand names of simulators will be avoided in this discussion. The software will be referred to by generic types.

In the **Simulator Verification and Validation** section of this manual, guidelines will be given for testing the capabilities of a selected simulator. Simulator inaccuracy may occur due to improper application, i.e. using a simulator for a problem for which it was not intended. One of the main objectives of this manual is to aid the user and evaluator in judging the proper simulator capability level required in certain problem applications. Since simulator codes are usually very long and complex, and since most codes are proprietary and not available for review, an indirect method of verification is normally required. This section discusses some test problems which may be used in verification. The details of these problems appear in an appendix to this manual.

The next section of this manual, **Data Requirements,** will discuss the specific information required by the simulator for each problem type. Criteria for minimum data requirements are given. Additional data, which would improve the results of the simulation, will be stated. Direct and indirect methods for gathering the desired data will be discussed.

The **Data Development** section of this manual deals with reducing the measured data to an appropriate form for use in the simulation. The

form of parameters required by the simulator is often influenced by the problem type, the simulator type, and the grid cell sizes. The very nature of the process of studying a volume of subsurface rock as an assortment of discrete blocks requires special treatment during the assignment of rock and fluid properties within these blocks. In addition, it is important that the approximate limitations of each parameter be known, as well as the cumulative effect these limitations may have on the simulation. This section of the manual gives guidelines for the analysis of all data required by the simulator or for the history matching process. Since it is expected that much of the needed data will often be unavailable, particular emphasis is given to methods of estimating the missing parameters.

After analysis of all data and determination of the required parameters, the derived information must be combined into a coherent description of the geology, and rock and fluid properties within the simulator. The **Model Construction** section of this manual discusses this procedure. The model consists of the simulator (computer code); the geologic, petrophysical and fluid descriptions; and the historical performance of any wells completed in the interval of study.

In the section on **Model Calibration,** the history matching process is discussed. In situations where historical performance data is available, it may be possible to corroborate the description of geology, rock, and fluids of the model by model performance. This section discusses the use and misuse of historical performance data in

calibration of the reservoir description. In addition, discussion of non-uniqueness of the data after completion of the history matching phase is discussed.

In most cases, the quantity and quality of the data available to define and calibrate the rock and fluid characteristics of the model are insufficient to provide a high degree of confidence in the simulation results. Many important parameters may have been estimated or may have wide ranges of accuracy. The **Sensitivity Analysis** section of this manual discusses determination of the effect of possible inaccuracies on the simulation results. By varying these poorly known parameters within their range of possible values, the effect upon the simulator's predictions can be determined. In this way, the critical parameters can be identified, a degree of confidence in the predicted results can be determined, and appropriate procedures for monitoring of the injection performance can be designed. The procedures for conducting and analyzing these sensitivity analyses will be described in this section of the manual.

In the **Prediction of Future Performance** section of this manual, guidelines are given for forecasting hazardous waste movement within the area of study. The discussion focuses on the design of simulation runs to determine whether migration of injected fluids out of the injection zone will occur. In addition, the interpretation of the results of these runs is addressed.

NATURE OF MATHEMATICAL SIMULATORS

To "simulate", as defined by Webster, is "to assume the appearance without the reality." Reservoir simulation provides us with a vehicle whereby the behavior of a reservoir (be it an aquifer or a hydrocarbon system) can be inferred from the behavior of a model which simulates it. A simulator becomes a specific model when geologic and fluid data are incorporated as input. The model could be a physical one (as constructed in a laboratory) or a mathematical one. We will confine our attention here to mathematical models. Within the mathematical category there are analytical models and numerical models. While there are a few situations for which exact analytical solutions are available, in general the resulting set of multi-dimensional partial differential equations which describe fluid flow in porous media are non-linear and may only be solved by a numerical approximation. In certain situations analytical models can be used. In particular analytical models can be utilized for single-phase, incompressible (or slightly compressible) unsteady-state fluid flow in porous media. We will utilize these analytical solutions directly wherever possible and indirectly in verification of numerical results. In general we will focus our attention upon the class of more flexible numerical models and the associated differences amongst them. Limited discussion will address direct use of analytical models and the associated assumptions governing their application.

HISTORICAL PERSPECTIVE

Models of one kind or another have been employed throughout the history of mankind. For the most part, they have been used to obtain a better understanding of the environment and to test the behavior of physical entities under the constraints of nature's laws. There has been an increasing dependence on models concurrent with the growth of petroleum and groundwater engineering technology. This dependence is unique and borders on total commitment inasmuch as the environment treated, the subsurface strata, is largely inaccessible.

For engineering purposes, a model is considered as an entity permitting the study of phenomena, under appropriate test conditions, that are likely to occur in practice. In this context, a model can be a physical device wherein one attempts to reproduce in microcosm the desired phenomena. On the other hand, it can take the form of physical concepts, expressed mathematically, from which one derives his conclusions by appropriate mathematical techniques. This is referred to as a "mathematical model".

Both physical and mathematical models have played an important role in the petroleum and groundwater industries. For example, the laws governing fluid flow in porous media were discovered and delineated employing physical models. Darcy's Law, the concepts of relative permeability, capillary pressure, density and viscosity correlations, and so on, all have their origins in experiments with physical

models. These models have been, and are, indispensible to the practice of reservoir engineering. Nevertheless, physical models have their limitations. These largely reside in the impracticality of rigorously modeling a large scale system. Such an undertaking would require surmounting formidable problems at prohibitive costs, and even then, the desired goal of obtaining a generalized physical reservoir model may not be attained. Physical models are most useful in studying phenomena on a small laboratory scale, and indeed are essential to determining the physical concepts controlling these phenomena.

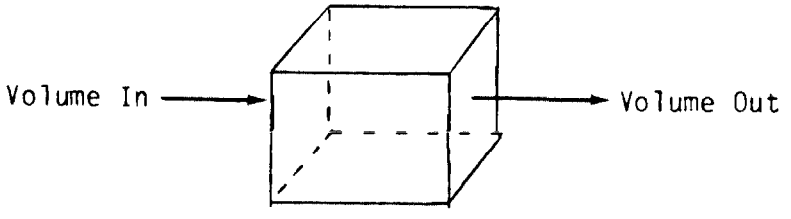
Modeling global systems requires a different approach, usually the mathematical one. The desire to adequately treat an entire reservoir with some degree of accuracy has given birth to the technology known as reservoir simulation. The term "reservoir", as used herein, applies equally to petroleum accumulations or aquifers. This is not to say that reservoir simulation techniques are limited to global situations. They are also used in studying local phenomena around wellbores, and have proven superior in this regard, to physical models.

Possibly only the name, "reservoir simulation", is new since the concepts involved have long been employed by reservoir engineers and hydrologists. Mathematical models, albeit simple ones, were devised beginning in the 1930's when reservoir engineering was still in its infancy. The most familiar of these is the material balance equation. This is a mathematical model or reservoir simulator in every sense. It is based on a fundamental physical concept, namely a

conservation principle. This principle, when expressed mathematically under the constraints of arbitrary assumptions, constitutes the model. It is worthwhile to note that modern reservoir models are based on the same principles. They differ insofar as attempts have been made to lift the restricting assumptions inherent in the material balance equation and more closely approximate actual subsurface conditions.

MATERIAL BALANCE EQUATION

The material balance equation was first introduced by Schilthuis (1936). He proposed treating a reservoir as a homogeneous tank having uniform rock and fluid properties throughout. Consequently, it is sometimes referred to as "the tank model". The tank is assumed sealed on all sides, i.e. it is a closed system with no flow across the boundaries. For this system, the conservation concept states that the volume of fluids entering the tank, less the volume leaving, equals the net change in volume. This is schematically depicted below:



Tank Model Concept

Since the tank is sealed, it is tacitly assumed the fluids are entering or leaving through injection and/or production wells (sources or sinks).

The equation that evolves from this treatment, and its various modifications, has been an important tool to the reservoir engineer. It has made possible estimations of fluids-in-place and the amount of fluid influx. Furthermore, it has provided means to predict oil production under various driving mechanisms such as solution gas drive, gas cap drive, etc. Another nice feature is that it yields a rather simple formula which an engineer can employ without resorting to a computer. Nevertheless, it has its drawbacks. These come into sharp relief when we compare the model to an actual reservoir.

First, the material balance equation (MBE) does not reflect the spatial variation of the rock and fluid parameters. Reservoirs actually are heterogeneous and anisotropic. Permeability, for example, changes from point to point (heterogeneity) and even at a given point, it may take on different values depending upon the direction (anisotropy). Values of porosity and the phase behavior of fluids, their densities, etc., also can vary appreciably throughout the reservoir. Another major deficiency of the MBE is that the actual geometrical configuration of the reservoir is not considered. This can have important ramifications where fluid flow processes are strongly affected by the reservoir geometry. For example, rapid segregation of fluids in high relief structures cannot be adequately modeled with the MBE. Furthermore, no provision is made to reflect the existence of wells and their locations within the system except to say that somehow fluids enter and fluids leave. Similarly, the dynamic effects (time dependence) of fluid movement within the reservoir

are neglected, and it is not possible to ascertain the spatial distribution of fluids with time. Thus, as one produces from or injects into the reservoir the shifting of fluid contacts cannot be predicted with the MBE. Nevertheless, the capability to do this is desirable for obvious reasons.

The deficiencies of the MBE were recognized early and a number of means were taken to overcome them. Some of these exploit physical models more fully. One approach employs the similarity between flow of electricity and fluid flow. This correspondence permits the development of an electrical analog of a reservoir using resistance-capacitance networks. Another approach uses a large container sculptured to conform to the boundaries of a reservoir. The container is filled with an aqueous electrolyte and individual wells are represented by copper electrodes placed within the system. Current fed to the electrodes simulates injection and production rates. The objective of the "potentiometric model" is to determine steady-state potential distributions and reconstruct locations of flood fronts. The biggest weakness in these approaches is that a unique model has to be custom built for each reservoir problem. The network analyzer furthermore is cumbersome and not readily adaptable as a general purpose simulator. The potentiometric model is also restricted to fluid flow regimes having unit mobility ratios and cannot reflect reservoir heterogeneities and anisotropies. Since the advent of numerical methods these approaches are now rarely, if ever, used.

MODERN NUMERICAL SIMULATORS

Attempts to construct a mathematical model that overcame the deficiencies of the MBE invariably arrived at equations that fall within the category requiring numerical solutions rather than analytic ones, hence the name "numerical simulators". The volume of work required to achieve numerical answers to even the simplest subsurface flow problems is astronomical. Consequently, high speed digital computers are relied upon to accomplish this task. Indeed, with the advent of high speed computing equipment, it is now possible to employ generalized simulators to study the behavior of many subsurface systems under a wide range of operating conditions.

In one sense, modern numerical simulators can be thought of as a group of contiguous MBE tanks which cover the area of interest. Obviously, the smaller the elements or blocks, the more accurately the reservoir geometry can be defined. Flow occurs across the faces of the interior blocks, but over each of these blocks the same conservation notion employed by Schilthuis is invoked, however, in slightly different form:

Mass of Fluid In - Mass of Fluid Out = Net Change in Fluid Rate

The collection of such material balance equations over each block constitutes the mathematical model.

The rate form has the advantage that it employs Darcy's Law and neatly introduces the dynamic effects of fluid movement. Furthermore, by segmenting the reservoir into a collection of small blocks, unique values of the rock properties can be assigned to each and thereby approximate subsurface heterogeneities and anisotropies can be modeled. Spatial variation of fluid properties can also be assigned blockwise or zonewise throughout the system. To reflect the existence of wells, appropriate source (for injection) or sink (for production) terms were added to the conservation equation for a given block in which the well occurs. Because flow is permitted across interior block boundaries, fluid front movements can be tracked, changes in fluid contacts can be monitored and dynamic changes in pressure and saturation distributions can be determined. In brief, this approach essentially removes all the shortcomings inherent in the MBE.

The mathematics of modern reservoir simulation consists of sets of non-linear partial differential equations which are the result of combining a conservation equation with a flow equation. In the case of fluid flow, the equation of continuity is combined with Darcy's law for flow in porous media. These equations are written at the "nodes" or intersections of a rectangular grid and as such represent material balances for each block, or cell, in the grid. Since the faces of these cells are connected to one another the amount of flow into one cell must equal the flows into neighboring cells plus the fluid accumulation due to changes in cell volume(s). In the case of heat flow, Fourier's law is combined with a conservation of heat equation and in

the case of solute transport Fick's law for diffusion (and dispersion) must be incorporated with a conservation equation. Along the edges of a model grid where the reservoir is non-existent because of a lack of reservoir thickness or permeability a "no-flow" boundary condition is imposed. At wells centered in a grid cell, a boundary condition is imposed for steady withdrawal or injection over a time step. The flow rate is proportional to the difference between the average cell pressure and the flowing bottomhole pressure of the well (Darcy's Law).

Examples of one-dimensional (linear), two-dimensional, and three-dimensional grids are illustrated in Figures 1, 2, 3, and 4. The unknown variables at the center of each cell are pressure and the saturation of each phase. In the case of single-phase systems where the injectant is miscible with the reservoir fluid, the unknowns will be pressure and the concentration of the injectant in the cell. Fluids move and concentrations change with time and distance depending upon the rate of injection at the wells. Even in a liquid-filled system there is enough elasticity to accommodate injected fluid. The results for a single-phase system at each time level (months or years) are the pressure distribution and the concentration distribution in the grid system. For multi-phase systems the phase saturation will also be unknown at each cell. We will begin by examining single-phase flow.

In single-phase flow the rock properties of permeability, porosity and thickness must be known and assigned initially for each cell. The

porosity of the system is the fraction of rock volume which is commonly called "pore volume" or the volume in which the fluid resides (see Figure 5). This space is also called the interstitial volume which is the void space between sand grains in a rock. This volume may be thought of as a three-dimensional "cob-web" of pores connected by pore throats. The pore throats are small capillaries or pipes which control the fluid movement from one pore to another in the reservoir pore space. The permeability of the rock is a quantification of the size and number of these pore throats that control fluid movement under a given pressure gradient. The thickness of a cell can be variable from cell to cell and may represent a complete rock layer or a single sand within a layer. If a system is completely homogeneous each cell may be assigned the same value of porosity and permeability. This situation is unlikely for most reservoir systems since some degree of heterogeneity is to be expected.

Other Simulation Approaches

Up to this point, the manual has concentrated on models that are based on numerical approximations to the diffusivity and advective-dispersive equations (which are solved using the method of finite differences). There are also other approaches to modeling ground-water flow and solute transport. Generally these fall into these three categories: analytical, semianalytical, and other numerical methods. Analytical and other numerical methods will be covered in this manual. For semianalytical methods, the reader is referred to Javandel, et al.(1984).

Analytical Approaches

An analytical model is a direct solution to a given differential equation which describes a physical process with initial and boundary conditions. For our purposes, we are dealing with fluid flow and solute transport in porous media. Analytical models have several advantages: 1) they are relatively easy and quick to use when compared to a complex numerical model, 2) when used in the appropriate situation, they can give an order of magnitude initial estimation relatively quickly, and 3) analytical models are also a good alternative to numerical models when data is limited. There are also several limitations associated with analytical models: 1) analytical models are not as flexible and realistic as numerical models, 2) analytical solutions are available only for certain idealized conditions and may not be applicable to a field problem with complex boundary and initial conditions, and 3) spatial or temporal variation of reservoir parameters such as permeability or dispersivity cannot be handled with analytical models.

Analytical solutions to the diffusivity and advective-dispersive equations have been solved for a variety of initial and boundary conditions or assumptions. Most solutions for single-phase fluid flow are based on the following assumptions: 1) nonleaky artesian (confined) aquifers, leaky artesian aquifers, or water-table aquifers, 2) uniformly porous aquifers, 3) uniformly fractured aquifers, 4)

aquifers of infinite areal extent, 5) aquifers with the same thickness throughout, 6) isotropic aquifers, 7) homogeneous aquifers, 8) isothermal conditions, and 9) fluids with constant density and viscosity. In comparison, most solutions for solute transport are based on the following assumptions: 1) homogeneous aquifers, 2) isotropic aquifers, 3) aquifers of infinite areal extent, 4) aquifers with the same thickness through-out, and 5) a steady-state flow field that is either radial or a constant regional value. The above listing of assumptions should not be considered as "cast-in-stone," as there are several analytical models that are not constrained by them. Javandel, et al.(1984), Walton(1984) and Earlougher(1977), all give analytical solutions for several different problem types. When using analytical models one should always confirm that the initial and boundary conditions of the analytical solution fit the type of problem (conceptual model) at hand.

Analytical models can be used for a variety of applications. For example the results of a numerical model can be compared to an analytical solution to validate the numerical simulator. This topic will be covered in more detail in a later section of this manual. Analytical models can also be used as an aid to model construction. This is done by testing the numerical model's sensitivity to time and spatial discretization and controls on numerical dispersion. In addition, analytical models can be used to help determine the type of problem that needs to be modeled. Simplified aquifer and injection well system evaluation can be done with analytical models. Analysis of

aquifer-test data is the most classic example of applying analytical models. Analytical models can also be used to estimate groundwater flow and transport parameters from field or laboratory data which can not be measured directly. These parameters must be estimated through inverse methods from the observed data. A simplified parameter sensitivity analysis can also be accomplished with analytical models. Analytical models are ideal for a Monte Carlo simulation used to estimate uncertainty. Several thousand runs of an analytical model can be conducted with relatively little computer time.

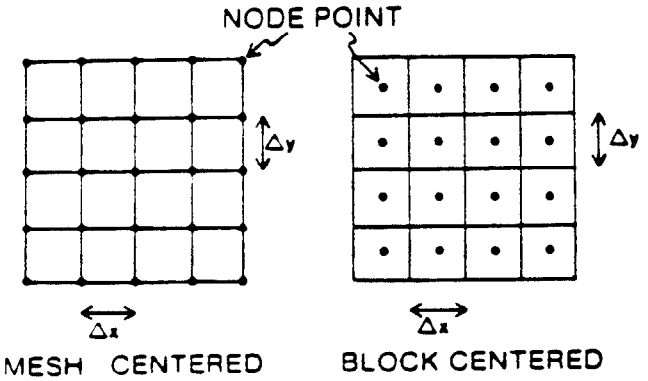
Several limitations of analytical models were mentioned above, and there are many ways of overcoming them. Due to the scope of this manual only the image-well theory will be covered. The image-well theory is a method where analytical models may be extended to model aquifers with finite areal extent. Briefly, the theory involves the use of a hypothetical image-well to model the effects of a hydrogeologic boundary on the cone of impression of an injection well. This theory will be more fully discussed, along with example problems, in the appendices to this manual.

Numerical Approaches

In addition to the popular finite difference method and the analytical solutions to the reservoir flow equations there is one additional method which should be mentioned. It is the finite element method. Mercer and Faust(1980) have written a series of papers about

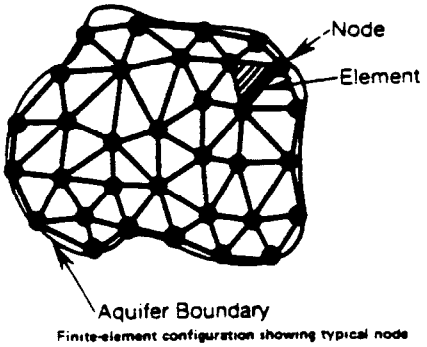
groundwater modeling which are recommended as additional background reading in the subject area; these authors point out that while the finite difference method is based on the method of differentiation (i.e. derivative representation by Taylor's series) the finite element method is based upon integration. Again the finite element method is more adaptable to the groundwater situation. One reason for this is that the relative permeability concept; two phases flowing at the same time at the same spatial location in a porous rock are difficult to formulate in the finite element approach. Therefore, while petroleum researchers have attempted solutions, only single-phase flow seems to be amenable, and research in the petroleum arena has continued to focus on finite difference methods.

In finite difference methods the set of partial differential equations are approximated over a regular rectangular or square grid. In the finite element method triangular shaped elements of varying dimension are often used for solution surfaces. The reader is referred to Mercer and Faust(1980) and the literature for more details. The different geometries for finite difference (a) and finite element (b) are depicted here.



Grids showing mesh-centered nodes and block-centered nodes.

(a)



Finite-element configuration showing typical node and element.

(b)

After Mercer and Faust(1980)

GROUNDWATER AND PETROLEUM NOMENCLATURE

Groundwater Hydrology

The radial diffusivity equation in groundwater form is:

$$\frac{\partial^2 h}{\partial_r^2} + \frac{1}{r}\frac{\partial h}{\partial r} = \frac{1}{0.1336805}\frac{S}{T}\frac{\partial h}{\partial t}$$

where:

h = hydraulic head, ft

r = radial distance from well, ft

S = storage coefficient, fraction

T = transmissivity, gals/(day/ft)

t = time, days

Petroleum

The radial diffusivity equation in petroleum form is:

$$\frac{\partial^2 p}{\partial r^2} + \frac{1}{r}\frac{\partial p}{\partial r} = \frac{1}{0.00026379}\frac{\phi \mu c}{k}\frac{\partial p}{\partial t}$$

where:

p = pressure, lbf/in^2

r = radial distance from well, ft

ϕ = porosity fraction

C = compressibility, psi^{-1}

μ = viscosity, centipoise

k = permeability, millidarcies

t = time, hours

Obviously the two equations have great similarity (After all it is the same equation!). In oilfield units, storage and transmissivity become

$$S = \phi c_t h \frac{\rho g}{g_c}$$

$$T = \frac{kh}{\mu}\frac{\rho g}{g_c}$$

$$\text{or } \frac{S}{T} = \frac{\phi \mu c}{k}$$

Three complete tables of groundwater and petroleum units for various equations and variables follows. The first two tables were taken from Monograph 7 of the Society of Petroleum Engineers by Robert C. Earlougher, Jr.(1977). The third table includes additional common units required for the conversion of hydraulic conductivity and transmissivity.

—COMPARISON OF UNITS AND EQUATIONS IN VARIOUS UNIT SYSTEMS *

Oilfield Units	SI Units	Preferred API Standard SI Units	cgs Units*	Groundwater Units
q — production rate, STB/D	m^3/s	dm^3/s	cm^3/s	Q — production rate, gal/min
h — formation thickness, ft	m	m	cm	m — formation thickness, ft
k — permeability, md	m^2	μm^2	darcy	—
μ — viscosity, cp	Pa·s	Pa·s	cp	—
k/μ — mobility, md/cp	$m^2/(Pa \cdot s)$	$\mu m^2/(Pa \cdot s)$	darcy/cp	P or K — coefficient of permeability, gal/day ft²**
kh/μ — mobility thickness product, md ft/cp	$m^2/(Pa \cdot s)$	$m(\mu m^2)/(Pa \cdot s)$	darcy·cm/cp	T — coefficient of transmissivity, gal/(day ft)**
Δp — pressure difference, psi	Pa	kPa	atm	s — drawdown, ft of water, >0 for pressure drawdown**
p — pressure, psi	Pa	kPa	atm	h — head of water, ft of water
r — radius, ft	m	m	cm	r — radius, ft
t — time, hours	s	h	s	t — time, days
ϕ — porosity, fraction				—
c_t — total system compressibility, psi⁻¹	Pa^{-1}	kPa^{-1}	atm^{-1}	S — coefficient of storage, fraction**
$\phi c_t h$ — porosity compressibility-thickness product, ft psi⁻¹	$m \cdot Pa^{-1}$	$m \cdot kPa^{-1}$	$cm \cdot atm^{-1}$	

DIMENSIONLESS TIME

$t_D = \dfrac{0.000263679\,kt}{\phi\mu c_t r_w^2}$	$t_D = \dfrac{kt}{\phi\mu c_t r_w^2}$	$t_D = 3.6 \times 10^{-4}\,\dfrac{kt}{\phi\mu c_t r_w^2}$	$t_D = \dfrac{kt}{\phi\mu c_t r_w^2}$	$\alpha = 0.1336805\,\dfrac{Tt}{Sr_w^2}$

DARCY'S LAW FOR INCOMPRESSIBLE, RADIAL FLOW

$q = \dfrac{0.00708188\,kh(p_e - p_w)}{B\mu \ln(r_e/r_w)}$	$q = 2\pi\,\dfrac{kh(p_e - p_w)}{B\mu \ln(r_e/r_w)}$	$q = \dfrac{2\pi \times 10^{-3}\,kh(p_e - p_w)}{B\mu \ln(r_e/r_w)}$	$q = 2\pi\,\dfrac{kh(p_e - p_w)}{B\mu \ln(r_e/r_w)}$	$Q = \dfrac{0.00436332\,T(h_e - h_w)}{\ln(r_e/r_w)}$

DIFFUSIVITY EQUATION

$\dfrac{\partial^2 p}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial p}{\partial r} = \dfrac{1}{0.000263679}\,\dfrac{\phi\mu c_t}{k}\,\dfrac{\partial p}{\partial t}$	$\dfrac{\partial^2 p}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial p}{\partial r} = \dfrac{\phi\mu c_t}{k}\,\dfrac{\partial p}{\partial t}$	$\dfrac{\partial^2 p}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial p}{\partial r} = \dfrac{1}{3.6 \times 10^{-4}}\,\dfrac{\phi\mu c_t}{k}\,\dfrac{\partial p}{\partial t}$	$\dfrac{\partial^2 p}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial p}{\partial r} = \dfrac{\phi\mu c_t}{k}\,\dfrac{\partial p}{\partial t}$	$\dfrac{\partial^2 h}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial h}{\partial r} = \dfrac{1}{0.1336805}\,\dfrac{S}{T}\,\dfrac{\partial h}{\partial t}$

GENERALIZED TRANSIENT FLOW EQUATION

$\Delta p = \dfrac{141.205\,qB\mu\,p_D(t_D)}{kh}$	$\Delta p = \dfrac{qB\mu\,p_D(t_D)}{2\pi kh}$	$\Delta p = 10^{3}\,\dfrac{qB\mu\,p_D(t_D)}{2\pi kh}$	$\Delta p = \dfrac{1}{2\pi}\,\dfrac{qB\mu}{kh}\,p_D(t_D)$	$s = 229.183\,\dfrac{Q}{T}\,p_D(\alpha)$

SLOPE OF SEMILOG STRAIGHT LINE

$m = 162.568\,\dfrac{qB\mu}{kh}$	$m = 0.183234\,\dfrac{qB\mu}{kh}$	$m = 1.83234 \times 10^{3}\,\dfrac{qB\mu}{kh}$	$m = 0.183234\,\dfrac{qB\mu}{kh}$	$M = 263.857\,\dfrac{Q}{T}$

GENERALIZED SKIN FACTOR EQUATION

$s = 1.15129\left[\dfrac{p_{1hr} - p(\Delta t = 0)}{m} - \log\left(\dfrac{k}{\phi\mu c_t r_w^2}\right) + 3.227546\right]$	$s = 1.15129\left[\dfrac{p_{1hr} - p(\Delta t = 0)}{m} - \log\left(\dfrac{k}{\phi\mu c_t r_w^2}\right) - 0.351378\right]$	$s = 1.15129\left[\dfrac{p_{1hr} - p(\Delta t = 0)}{m} - \log\left(\dfrac{k}{\phi\mu c_t r_w^2}\right) + 5.092319\right]$	$s = 1.15129\left[\dfrac{p_{1hr} - p(\Delta t = 0)}{m} - \log\left(\dfrac{k}{\phi\mu c_t r_w^2}\right) - 0.351378\right]$	$\text{skin} = 1.15129\left[\dfrac{s_{1hr} - s(\Delta t = 0)}{M} - \log\left(\dfrac{T}{Sr_w^2}\right) + 0.522555\right]$

*The cgs system is considered to be obsolete and is replaced by SI. cgs units are included only for comparison with published material. SI is a coherent system, so equations do not contain units conversion factors.

—RELATIONSHIP OF COMMON GROUNDWATER AND OILFIELD QUANTITIES.

A consistent-unit system is assumed. Variable definitions for each system are given in Table A.7.

Groundwater Quantity		Oilfield Quantity
Coefficient of permeability	$= P = K$	$= \frac{k}{\mu}\left(\frac{\rho g}{g_c}\right)$
Transmissivity	$= T = Km$	$= \frac{kh}{\mu}\left(\frac{\rho g}{g_c}\right)$
Coefficient of storage	$= S$	$= \phi c_t h\left(\frac{\rho g}{g_c}\right)$
Drawdown	$= s$	$= \frac{p_i - p}{(\rho g/g_c)}$
Head	$= h$	$= \frac{p}{(\rho g/g_c)}$
Dimensionless drawdown	$= W(1/4\alpha)$	$= 2p_D(t_D)$

CONVERSION TABLE FOR HYDRAULIC CONDUCTIVITY UNITS

	cm/sec	m/sec	m/day	ft/sec	ft/day	gpm/ft^2	gpd/ft^2
1 cm/sec	1.000	1.000×10^{-2}	864.0	3.281×10^{-2}	2.835×10^{3}	14.72	2.121×10^{4}
1 m/sec	1.000×10^{2}	1.000	8.640×10^{4}	3.281	2.835×10^{5}	1.472×10^{3}	2.121×10^{6}
1 m/day	1.157×10^{-3}	1.157×10^{-5}	1.000	3.797×10^{-5}	3.281	1.704×10^{-2}	24.54
1 ft/sec	30.48	30.48×10^{-2}	2.633×10^{4}	1.000	8.640×10^{4}	4.488×10^{2}	6.464×10^{5}
1 ft/day	3.528×10^{-4}	3.528×10^{-6}	3.048×10^{-1}	1.157×10^{-5}	1.000	5.194×10^{-3}	7.480
1 gpm/ft^2	6.791×10^{-2}	6.791×10^{-4}	58.67	2.228×10^{-3}	1.925×10^{2}	1.000	1.440×10^{3}
1 gdp/ft^2	4.716×10^{-5}	4.716×10^{-7}	4.075×10^{-2}	1.547×10^{-6}	1.337×10^{-1}	6.944×10^{-4}	1.000

CONVERSION TABLE FOR TRANSMISSIVITY UNITS

	m^2/sec	m^2/day	ft^2/min	ft^2/day	gpm/ft	gpd/ft	darcy · ft/cp
1 m^2/sec	1.000	8.64×10^{4}	6.459×10^{2}	9.301×10^{5}	4.831×10^{3}	6.957×10^{6}	3.413×10^{5}
1 m^2/day	1.157×10^{-5}	1.000	7.476×10^{-3}	10.76	5.592×10^{-2}	80.52	3.950
1 ft^2/min	1.548×10^{-3}	1.338×10^{2}	1.000	1.440×10^{3}	7.480	1.077×10^{4}	5.284×10^{2}
1 ft^2/day	1.075×10^{-6}	9.289×10^{-2}	6.944×10^{-4}	1.000	5.194×10^{-3}	7.480	3.669×10^{-1}
1 gpm/ft	2.070×10^{-4}	17.88	1.337×10^{-1}	1.925×10^{2}	1.000	1.440×10^{3}	70.64
1 gpd/ft	1.437×10^{-7}	1.242×10^{-2}	9.284×10^{-5}	1.337×10^{-1}	6.944×10^{-4}	1.000	4.906×10^{-2}
1 darcy ft/cp	2.930×10^{-6}	2.532×10^{-1}	1.892×10^{-3}	2.725	1.416×10^{-2}	20.38	1.000

CONVERSION TABLE FOR HYDRAULIC CONDUCTIVITY & INTRINSIC PERMEABILITY UNITS FOR WATER AT 20° C

	cm/sec	ft/day	gpd/ft^2	cm^2	darcy
1 cm/sec	1.000	2.835×10^{3}	2.121×10^{4}	1.027×10^{-5}	1.040×10^{3}
1 ft/day	3.528×10^{-4}	1.000	7.480	3.623×10^{-9}	3.669×10^{-1}
1 gpd/ft^2	4.716×10^{-5}	1.337×10^{-1}	1.000	4.842×10^{-10}	4.906×10^{-2}
1 cm^2	9.740×10^{4}	2.761×10^{8}	2.065×10^{9}	1.000	1.013×10^{8}
1 darcy	9.613×10^{-4}	2.725	20.38	9.870×10^{-9}	1.000

PROBLEM TYPES/SIMULATOR SELECTION

In hazardous waste injection, there are an extremely large number of possible combinations of geology, rock properties, in situ fluid properties, and injected fluid compositions. However, these combinations can be reduced to a relatively small number of "problem types." In general, any situation within a given problem type, can be modeled with a particular type of simulator. The definition of problem types and the selection of an appropriate simulator for a given problem will be discussed in this section.

One must consider the chemical nature of the injectant and in situ fluids and the geologic nature of the reservoir rock when determining problem types and selecting the type of model to use. Once the physical attributes of the problem are considered one can examine the simulator to see if it incorporates the proper mechanisms to model the reservoir. If one is unsure of the importance of any given variable upon the model results, sensitivity studies over expected ranges of the variable may be performed to see how the results change. In this way the primary variables can be identified.

The problem type can generally be defined by the following criteria for hazardous waste injection:

- model dimensions
- fluid phases/miscibility

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The problem type can generally be defined by the following criteria for hazardous waste injection:

- model dimensions
- fluid phases/miscibility

- single/dual-porosity
- fault treatment
- diffusion
- hydrodynamic dispersion
- chemical reactions
- thermal effects

The following section will discuss the use of these criteria in determining the particular problem type.

MODEL DIMENSIONS

As described in the previous section of this manual, the simplest simulation problem is a one-cell or tank model. This type of model is useful in testing simulator calculations against an analytic solution. For example, material balance calculations can be checked. More complex processes, such as dissolution and miscibility can also be tested. However, except in simulator verification and basic process testing, the one-cell model has little use in reservoir simulation. As discussed previously, multi-dimensional models are required to simulate the effects of heterogeneity and anisotropies on reservoir behavior.

The next simplest modeling problem is the one-dimensional simulation. This type of model is sometimes used to analyze pressure tests. It is common to run pressure tests (pressure drawdown) or shut-in tests

(pressure buildup) in single wells. There are several USGS publications dealing with this subject; Stallman(1976), Bennett(1976) and Reed(1980). If one assumes the aquifer layer to be vertically homogeneous in porosity and permeability, then a one-dimensional, radial problem will provide a satisfactory simulation (Figure 6). During a pressure test, the bottomhole pressure vs. time is tabulated. By performing the same test on the one-dimensional model, a calculated pressure vs. time curve will be developed which represents that of the actual well test. If reservoir parameters are estimated and adjustments are made until values are determined at which the model pressures match the actual data, a simple "history match" has been performed.

The next level of complexity would be represented by two-dimensional cross sections (Figure 7) and two-dimensional areal models (Figure 8). These may include one well or several wells. Density differences between injectant and in situ fluids may cause gravity segregation in the two-dimensional cross section problem. The effect of variations in reservoir properties areally on fluid flow can be simulated using the two-dimensional areal model. These types of models can be utilized to study the details of certain processes or to simulate flow within reservoirs in special situations. However, most problems encountered in the injection of hazardous wastes will require more definition than a two-dimensional model can provide.

Full three-dimensional simulations will be most prevalent in understanding complete reservoirs. These models will include overburden

and underburden confining layers so that vertical migration can be evaluated. If sufficient geological data is available these models can be divided into several vertical layers.

FLUID PHASES/MISCIBILITY

When injecting an aqueous waste into an aquifer the resulting mixture is usually miscible, i.e. the waste will mix with the aquifer in all parts. The result is a single-phase system. In single-phase systems the objective is to track the injected hazardous waste constituents so that its advance throughout the system can be predicted.

Only single-phase systems and the various phenomena associated with single-phase fluid systems in reservoir rocks have been considered in prior discussions. An additional order of complexity occurs if the injected waste is not miscible (i.e. immiscible) with the in situ aquifer fluid. This complication may occur if the injected waste is a hydrocarbon solvent or some other solvent which will not mix in all parts with aquifer water.

With the addition of a second phase, the simulator will have to accommodate relative permeability and capillary pressure effects. Relative permeability curves are illustrated in Figure 9. Capillary pressure curves are shown in Figure 10. Note that there are saturations of each phase below which no flow of this phase can occur (S_{orw}). This means that as solvent is injected some of it will become immobilized due to this principle.

CONCENTRATION EFFECTS

When injecting waste into an underground saline aquifer the simulation will be for a single-phase miscible fluid. Within this single fluid phase the simulator should contain a provision for tracking the concentration of waste in each grid block. Normally concentrations are expressed as C/C_o where C_o is the injected concentration and contains units, lbm/ft^3 or similar, and C/C_o is dimensionless. The simulator can be initialized with $C/C_o = 0.0$ in all reservoir blocks and the injection wellstream is specified at $C/C_o = 1.0$. By observing concentration maps at various time steps we can observe the frontal advance of the waste; C/C_o at any spatial location.

In addition to tracking the concentration, the simulator should contain mixing rules for obtaining the viscosity and density of the fluid mixture. In most cases the viscosity of the injectant will probably be nearly the same as water since dilute solutions are usually injected. In any case where the viscosity of the injectant is less than the resident water it is possible to have "fingering" of injectant due to unequal mobilities of the injectant and in situ water. Mobility is expressed as k/μ , permeability/viscosity ratio. If the simulator correctly addresses dispersion (discussed later), and mixing rules are included, the viscosity of the fluid mixture should be taken care of in the course of the explicit (between time step) fluid property calculations. It is not expected that many problems will need to be concerned with viscosity mixing.

Density mixing is handled similarly, utilizing grid block concentration values. Concentration maps can be either volume fractions or mole fractions. Mixing rules are usually developed on the same basis, simply weighting the fluid property of interest by its mole fraction in the grid block and summing the weighted fluid property for the two components. An injected fluid of higher density will "under-run" the in situ fluid due to gravity effects. "Over-running" of the injected fluid will occur if the injected fluid is of lower density. These effects will probably be subtle in most cases since the density contrast will probably be only slight. Over long periods of time, however, the contrasting effect on the spread of the waste front could be significant. The effects of density contrast will be greater in thick intervals of an aquifer where all layers are in communication vertically.

SINGLE/DUAL POROSITY

One of the most important, and sometimes most difficult, decisions to be made when performing a simulation study, is whether the reservoir will behave as a single- or dual-porosity system. A single-porosity system is one in which there are no large heterogeneities in effective permeability in either a vertical or horizontal direction. It is recognized that vertical permeabilities may be anywhere from 5% to nearly 100% of the value of horizontal permeabilities. In a single-porosity system, the pore volume behaves as though it is all connected as a single pore volume. Examples of these types of systems range from truly homogeneous reservoirs, such as clean beach sands, to

reservoirs whose properties vary in a relatively smooth manner vertically and areally.

On the other hand, in a dual-porosity system, there exist two or more sets of pore volumes with significantly differing effective permeabilities. A familiar example is that of a porous rock matrix containing highly permeable fractures. In this case the fracture permeability is often quite high, on the order of thousands of millidarcies. The rock matrix may have as little as 50-100 md or less in a carbonate matrix. A dual-porosity simulator is definitely required to model a fractured system. Figure 11 contains an illustration of a fractured reservoir and a schematic of a reservoir model for a dual-porosity system.

Another example of a dual-porosity system is a stratified reservoir with high permeability contrast between reservoir layers. If a highly permeable layer is connected vertically to a low permeability layer, and in addition if a wellbore penetrates only the highly permeable layer, then reservoir pressure response will behave as a dual-porosity system. In this case, however, a single-porosity simulator will most likely suffice in most instances. The reason for this likelihood is that the different strata can be represented with correct permeability and porosity values and the frequency of occurrence of the contrasting permeability/porosity medium is of finite frequency. This attribute is not true of frequently occurring natural fractures interspersed in matrix rock in a fractured system. In the true naturally fractured

case, the reservoir behaves as a parallel network of matrix rock connected to a second network of fractures. Even if a second network of thin layers could be included in a single-porosity simulator to represent the fracture network, computing efficiency would be extremely poor. The need for improved computing efficiencies, among other technical reasons, is the reason why this second class of dual-porosity simulators has come into being.

One difficulty in determining the type of system one is dealing with, can result from the discontinuity or isolation of the secondary system. For example, if few wells have been drilled, it is possible to have overlooked discontinuous high permeability sand lenses or nearly vertical fracture planes. There are essentially four sources of information which are useful in determining if a formation, or set of formations, represent a single- or dual-porosity system. These are:

- well logs
- core analyses
- pressure tests
- well performance

Well logs, which measure reservoir characteristics, can often give evidence as to whether two or more distinctly different systems are present. However, as logs do not directly measure permeability, the evidence provided is normally not conclusive. However, log analysis

data combined with other information, such as well performance or core data, can provide correlations between logs and other permeability data. One type of log, developed for the petroleum industry is advertised as a "fracture identification" tool. However, these tools do not actually identify fractures but rather discontinuities in the reservoir, and their results should be viewed as such.

Core analyses, on the other hand, can provide direct evidence for single- or dual-porosity systems since permeabilities can be measured and fractures can be observed. As with well logs, core analyses are useful only as they are representative of the reservoir. Since they only sample the reservoir at a single-point, it is possible to be unaware of dual-porosity features a short distance away. Care should be taken to distinguish between natural fractures and those induced during drilling or analysis. In addition, some fractures are not highly permeable and may actually form permeability barriers if mineral deposits have formed along the fracture face.

Probably the best evidence for single- or dual-porosity systems is derived from long duration well tests. Methods exist by which pressure buildups, fall-offs, or interference tests can be analyzed to determine the type of system present, and important parameters of each system such as flow conductivity, storativity, and interporosity flow parameters. In addition, the well does not have to intersect all systems. The only requirement is that both natural fractures and matrix rock be in the radius of investigation of the test.

As a last resort, well performance data can give clues to the existence of single- or dual-porosity systems. High productivities from wells with poor characteristics from log and core analyses often suggests the presence of fractures. Flow meter measurements are useful in identifying the source of the flow. In addition, the production of water, oil, or free gas from a completion interval which is far from a source of any of these phases may suggest flow through high permeability conduits.

Simulation of relatively homogeneous reservoirs does not require special simulators or simulation techniques. The number of layers and number of cells areally will depend upon the expected injection/production rates, the presence of flow barriers, and the information required as results. In some cases, dual-porosity systems can also be simulated using single-porosity simulators. A representative example occurs when the primary and secondary systems are layers of differing permeabilities. By adapting the layering of the simulator to match that of the stratigraphy, the two-porosity system will be well represented by a single-porosity simulator.

However, some situations exist which are not accurately modeled by standard single-porosity simulators. These basic simulators will not rigorously simulate most fractured reservoirs. In order to simulate these reservoirs accurately it is necessary to represent the properties of both the matrix and fracture system for each grid cell. In order to track the movement of fluids, it is also necessary to compute

the couplings between these two systems at each grid cell. Attempts have been made to model fractured reservoirs with a single-porosity model. However, these attempts have required unnatural reservoir descriptions, required greatly increased computational time, and only resulted in poorly approximated representation of flow behavior at best.

Many modelers feel that when dealing with a fractured reservoir without information on the extent and nature of the fractures, that using a dual porosity model is not warranted in these situations. These modelers address this problem with a single porosity estimation of the fractured reservoir. Dealing with fractured reservoirs in this manner will result in predictions that have a large uncertainty associated with them. Single-porosity models can both over-predict and under-predict the maximum extent of a waste plume. Over-prediction is the result of not accounting for diffusion of solute from the fracture into the matrix. Under-prediction can result if waste is being transported large distances in natural fractures and the model is a single-porosity model.

FAULT TREATMENT

Consider the situation in Figure 12. Because of the displacement of corresponding geologic strata on either side of the fault there may be some difficulty in modeling fluid flow across the fault. One has to decide at the outset of course, whether or not the fault allows trans-

port of fluids across it. Information from geologists who are familiar with the post-depositional geologic history should help in this regard.

Some faults may be mineralized over geologic time and may not allow any or only partial fluid transport across them. Other information which may help in the decision is to see if a pressure interference test can be run between wells on either side of the fault. Simulators which can accommodate this situation properly usually have a section in the user's manual describing the treatment of fault-linkage. This problem is not a trivial one and, unless handled properly, can cause aberrant results in the simulation. With respect to hazardous waste the aspect of leakage is particularly important when considering storage in reservoir media containing faults.

HYDRODYNAMIC DISPERSION

The underground injection of hazardous waste, for the most part, is a single-phase, miscible displacement problem. The task of predicting the location, or spreading, of injected waste becomes one of tracking the transport of dissolved hazardous constituents. The most widely used mathematical description of the solute transport process is the advection-dispersion model. Advection is analogous to the concept of plug flow or the calculation of a waste front based on the average pore water (interstitial) velocity. Dispersion, or hydrodynamic dispersion, is the spread of the waste front due to differing pore-water velocities. Termed mechanical mixing, dispersion, in addition

to molecular diffusion can contribute significantly to the spread of waste.

The extent of mechanical mixing is a function of the groundwater velocity plus the velocity imposed from injection of waste. Mechanical mixing will be referred to as dispersion for the rest of the manual.

Stalkup(1983) gives a useful example in Figure 13 of dispersion resulting from microscopic mixing. Individual streamlines 1, 2, and 3 carry differing compositions at different pore velocities. As these different compositions pass through the rock, mixing cells are created at a, b, c, and d. As the fluids emerge from each of these cells they are of uniform (but different) compositions. The injected composition is dispersed both in the direction of flow (longitudinal) and transverse (orthogonal) to the direction of flow.

Dispersion causes the spread of injected waste to be accelerated beyond that expected by bulk flow alone. Therefore, any simulator not including dispersion will underestimate the rate and extent of the spread of injected waste if miscible dispersion is expected to occur.

Further complications occur for the interface between neighboring rock layers both of which are transporting injected waste. Stalkup(1983) also illustrates such a case in Figure 14. From this figure one can obtain a feel for the additional spread caused by transverse and longitudinal dispersion between injected waste and in situ water.

Longitudinal dispersion contributes to the smearing of the mixing zone interface in the principle direction of flow (normally in a perpendicular direction away from the wellbore). Transverse dispersion occurs between rock layers or intervals where flow in one layer is proceeding at a higher velocity than in an adjacent layer. The reader may refer to Figure 14 to reinforce these verbal descriptions. Transverse dispersion coefficients are normally 3-10% of the magnitude of longitudinal dispersion coefficients.

These conclusions about longitudinal and transverse dispersion lead us to another important realization. Dispersion is most important in lateral spread of waste away from the wellbore. The lateral intermixing of waste with in situ waters (along the bedding planes of the rock) will be responsible for the widest spread of waste because velocities are highest in the longitudinal direction.

The measure of the amount of mechanical mixing that takes place in an aquifer is known as the dispersivity. Methods used to obtain this important parameter will be discussed in a later section. Dispersivity has been the topic of several research studies in recent years. Several researchers have noted an apparent scale and time dependency associated with full aquifer dispersivities [Pickens and Grisak, (1981a), Pickens and Grisak,(1981b)]. In addition, several researchers have noted that field scale dispersivities are an order of magnitude greater than dispersivities measured in laboratory experiments (Anderson, 1979). A series of papers done by researchers at Auburn

University(Molz, et al., 1983; Guven, et al.,1984; Guven, et al.,1985) have shown that the above problem with full aquifer dispersivities can be explained by the heterogeneous nature of aquifers. Figure 22 shows an idealized example of a horizontally stratified aquifer. Each layer of the aquifer has a different permeability. Waste injected into such an aquifer will be transported not as a vertical straight line front, but as a front with fingers of different lengths extending out into the aquifer. If one were to measure the concentrations of the aquifer with fully penetrating wells and calculate the full aquifer dispersivity, the result would be based on an integration of the different waste concentration from each layer. This will result in a dispersivity that is much larger than the dispersivity of any individual layer. The full aquifer dispersivity measured by this method will change with increasing distance from the injection well and increasing time of injection.

Modeling the advancement of the waste front with full aquifer dispersivities becomes a complex problem, which some researchers have tried to do with dispersivities that change with time and distance. An additional erroneous effect of modeling an injected waste front with full aquifer dispersivities is that the real concentrations in the aquifer will not be accurately predicted. Studies have shown that the most important parameter in predicting the transport of waste away from the wellbore is not dispersion but a detailed description of the heterogeneous and isotropic distribution of permeabilities and porosities in the injection zone. Petitioners who model injection well

sites with limited amounts of data using assumptions of full aquifer dispersivities and homogeneous and isotropic hydraulic properties will have to be careful not to under-predict the maximum extent of the waste front on the site. Such predictions will have a greater amount of uncertainty associated with them.

Our other concern involves leakage into aquitards. Since transverse dispersion is small (3-10% of the magnitude of longitudinal dispersion), and since dispersion is a velocity dependent function and leakage velocities are low, we need not be concerned about dispersion in leakage calculations; convection alone will suffice for most cases.

CHEMICAL REACTIONS

The petrophysical fabric of subsurface rock is complicated and extremely variable. In general, there are two common types of reservoir rocks: sandstones and carbonates. Siltstone and shales generally lack the required permeability or effective porosity to be classified as reservoir rock. The same can be said for nearly all igneous or metamorphic rocks. The composition of the fabric of reservoir rocks may include quartz, feldspars, clays, anhydrites, dolomites, and various cements, to name a few. The chemistry of the groundwater resident within any particular rock is often indicative of the chemistry of the rock itself; i.e. the aquifer is likely to be in ionic equilibrium with the rock. Under these circumstances any upset in the chemical equilibrium can cause disintegration of clay particles due to

ion exchange or any number of other reactions. If the rock permeability is low enough, serious degradation can be caused by the movement of these particles. Pore throats may become plugged with clay fragments thus reducing permeability.

In addition to the upset in chemical equilibrium of aquifer/rock systems, other phenomena such as adsorption may take place. Figure 15 is an adsorption isotherm for petroleum sulfonate. Injected chemicals may adsorb to rock surfaces due to chemical and/or physical adsorption. This may in fact be advantageous if immobilization of hazardous waste is useful in the storage cycle. However, reductions in permeability, and thus injectivity, may occur.

Chemicals in certain types of injected wastes may also react to form precipitates within the aquifer. Iron and/or barium compounds are known to precipitate when injected fluids are incompatible with the in situ water.

It is not the purpose of this manual to provide a complete discourse on these subjects, rather it is our purpose here to draw the reader's attention to the complex chemical phenomena which may occur upon injection of hazardous waste. In some cases it may be desirable to form precipitates and/or have injected chemicals adsorb to rock surfaces in order to render the injected chemical immobile. In addition, in situ reactions may change the chemical form of the injectant to something less hazardous.

In general, all of the aforementioned reactions would seem to generate a desirable result; i.e. render the hazardous chemical immobile or transform it to something less hazardous. Precipitates or changes in clay chemistry often reduce reservoir permeability levels and may eventually cause impairment of the wellbore sandface if in situ permeability levels are low to begin with. Any reservoir simulator incapable of modeling reaction kinetics will, most likely render a pessimistic result in that injected waste may be transported too far and spreading will be greater in extent than will actually occur.

The real answer in all of these questions lies in laboratory coreflooding with appropriate measurements of ionic levels of important constituents into and out of the core. Clays can often be stabilized by adding potassium and/or calcium to injected fluids.

THERMAL EFFECTS

Most chemical reactions are completed at a faster rate at elevated temperatures. This result is mathematically described by the Arrhenius equation:

$$K = K_o e^{-A/RT}$$

where:

K_o = reaction constant at some base temperature, T_o
K = reaction constant at temperature T
A = activation energy
R = universal gas constant
T = absolute temperature

When graphed as ln K vs. 1/T the function is a straight line of slope -A/R. Small changes of temperature can cause orders of magnitude change in the rate of reaction.

The geothermal gradient of the earth's subsurface varies but in general is 1-1.5° F/100 ft. of depth. If a disposal well is perforated in a deep aquifer, say 10,000 ft subsurface, the temperature could easily be 160-200° F. If the hazardous waste contains components reactive with either the rock or components of the aquifer brine one can expect those reactions to proceed at elevated rates.

If a precipitate is being formed the reduction in near wellbore permeability may be disastrous and the well may have to be abandoned. If the waste stream contains any bacteria and oxygen the growth rate of the bacteria in the warm underground reservoir may also plug the formation. Surface treatment of the waste with chlorine or some other chemical may be required to kill the bacteria before injecting it underground.

Knowledge of these effects can be utilized in selecting a waste storage system or in effecting a non-hazardous degradation; however one should understand the effect of temperature upon any anticipated chemical reaction between the hazardous waste and geochemical constituents of the water and/or rock fabric.

SUMMARY OF PROBLEM TYPES

Problem type can generally be categorized by the following three major criteria:

- Injectant Type
  - Aqueous (miscible with aquifer water)
    - Diffusion/Dispersion
    - Chemical Reactions
    - Concentration Effects (density, viscosity)
    - Thermal Effects
  - Immiscible Solvent
- Geology Type
  - Single-Porosity (unfractured rock)
  - Dual-Porosity (fractured/fissured rock)
  - Faults
  - Stratification (multiple layers)
- Geometry
  - Single Dimension
  - Multiple Dimensions

Proper definition of the problem type will normally characterize the type simulator required. Some discussion is in order so that we may elaborate.

Injectant Type

Injectants are either aqueous based or solvent based. If the injected waste is a dilute water solution of hazardous waste it will be miscible with the aquifer water. In other words only a single-phase simulator capable of tracking the concentration of waste components in aquifer water is necessary. The tracking of compositions or concentrations may be required for more than one species if there are chemical reactions involved.

If velocities are high the capability of the simulator in handling dispersion may be necessary.

If chemical reactions are present and the temperature of the aquifer is higher than the injected waste then the ability to calculate the effect of temperature on the mixture may be important.

The prior statements pertain to solvent-based waste as well. In addition if the waste is solvent-based, the problem requires relative permeability curves for each phase as well due to immiscibility.

Geology Type

Unless the storage reservoir is known to be fissured or naturally fractured a single-porosity model is most likely all that is required.

If faults are occasionally encountered, one needs to know if the simulator can link different model layers to one another across faults; i.e. if displacement is great enough, lithology layer 2 may be connected with lithology layer 4, etc. Some simulators can accommodate this problem; some can not.

The capability to handle multiple layers or strata is fundamental. In most cases several layers within the zone of injection will exist, not to mention the over- and under-burden layers which are hoped to be containment barriers. Even shales and other so-called "sealing" strata have some permeability, even if it is 10^{-3} millidarcies or lower. Over 10,000 years even these will theoretically leak to some degree.

Geometry

It is difficult to imagine a situation where less than three dimensions are adequate. Perhaps symmetry can be assumed in one dimension thereby reducing the problem to 2-D. Occasionally one dimension could be adequate; such may be the case with pinnacle reefs or single-well problems in which the injection zone is truly homogeneous.

SIMULATOR SELECTION

Once the problem type characteristics are defined choosing a simulator becomes a straight-forward exercise. One must match the problem type requirements with simulator capabilities.

The following section contains a table, entitled "Simulator Complexity," which illustrates several choices for a single-porosity simulator. The same cases may be repeated for a dual-porosity simulator.

Our best estimate of the most widely used simulator for waste disposal problems will be the 3-D simulator designated*. The second most widely used simulator will add chemical reactions to the first.

SIMULATOR DESCRIPTION

The following list should be provided with each petition in order that a complete description of the simulator is received.

1. name of code/model/simulator;
2. name of the code/model/simulator's developer;
3. is the code/model/simulator proprietary;
4. purpose of the code/model/simulator;
5. the physical processes the code/model/simulator is simulating;
6. governing mathematical equations, and underlying assumptions;
7. method used to solve the equations, and limiting conditions resulting from the chosen method;
8. boundary conditions that can be incorporated in the code/model/simulator;
9. is a user's manual available;
10. a report on the verification and validation of the code/model/simulator; and

11. inclusion of any publication and or peer review articles on the code/model/simulator.

SIMULATOR COMPLEXITY

* **Single Porosity (Unfractured)**

	Dimensions	Phases	Wells	Diffusion/ Dispersion	Chemical Reactions	Fractures-Dual Porosity/Permeability
Simplest	1**	1	1	No	No	No
	1	1	1	Yes	No	No
	1	1	1	Yes	Yes	No
	2	1	>1	No	No	No
	2	1	>1	Yes	No	No
	2	1	>1	Yes	Yes	No
	3	1	>1	No	No	No
Most Widely	3*	1	>1	Yes	No	No
Applicable	3	1	>1	Yes	Yes	No
	3	2	>1	No	No	No
	3	2	>1	Yes	No	No
	3	2	>1	Yes	Yes	No
	3	3	>1	No	No	No
	3	3	>1	Yes	No	No
Most Complex	3	3	>1	Yes	Yes	No

---

* **Dual Porosity (Fractured)**

Simplest	1	1	1	No	No	Yes
	1	1	1	Yes	No	Yes
	1	1	1	Yes	Yes	Yes
	2	1	>1	No	No	Yes
	2	1	>1	Yes	No	Yes
	2	1	>1	Yes	Yes	Yes
	3	1	>1	No	No	Yes
Most Widely	3	1	>1	Yes	No	Yes
Applicable	3	1	>1	Yes	Yes	Yes
	3	2	>1	No	No	Yes
	3	2	>1	Yes	No	Yes
	3	2	>1	Yes	Yes	Yes
	3	3	>1	No	No	Yes
	3	3	>1	Yes	No	Yes
Most Complex	3	3	>1	Yes	Yes	Yes

* For full-blown (commercial) hazardous waste disposal problems it is expected that this case will be the most widely applicable. If data are available for reaction kinetics the most desirable simulator would be this one with the addition of chemical reactions.

** This simulator will be most widely utilized to match pump tests and develop formation flow capacities, kh in md ft.

SIMULATOR VERIFICATION AND VALIDATION

PREFACE

There are two chapters in this manual which involve the testing of the simulator and the resulting model as to the validity of the representation of the actual site specific problem by the model. There are two components to the question of validity; 1) is the mathematical capability of the simulator comprehensive and accurate enough, and 2) is the available data set adequate to represent the site specific description. We have chosen to discuss these issues in two parts; we discuss the verification and validation of the simulation code here and the model calibration in a later chapter. Finally, a chapter about sensitivity analysis follows the model calibration chapter for situations where little historical injection data and/or geologic data are available for calibration.

The process of validation as approached herein is comprehensive in that our interest lies in the application of a simulator to a hazardous waste injection site. Considering the various parts of this process we must not only be sure that the simulation code is verifiable, i.e. mathematically accurate, but that all geological, petrophysical, and fluid data have been researched and correlated into a proper geological description. Finally all historical injection data (rates and pressures or heads) should be utilized in the final calibration of the existing model (simulator plus input data).

Because of the complexity of this comprehensive process the end result, i.e. the application, will be no stronger than the weakest of its component parts (simulator, digestion of geological data, and final calibration). Because it is this final application that is of interest the knowledge and past experience of the engineers, hydrologists, and geologists/petrophysicists involved in the model development and application is important. A simple simulator, be it analytic or numeric in basis, in the hands of an accomplished technologist may well produce a better result than the most sophisticated simulator in the hands of an inexperienced person.

Because of the integrated nature of the application one must view each part of the process as to its validity and robustness. This section and the following sections discuss simulator verification, data requirements and development, model construction and calibration, sensitivity analyses and prediction of future performance. As a petition is prepared and reviewed one should be able to identify and judge the adequacy of each part of the process.

GENERAL

Van der Heijde, et al.(1985) have given guidelines as to the proper technique for testing and validation of groundwater models. These techniques were developed at the Holcomb Research Institute International Groundwater Modeling Center at Butler University in Indianapolis, Indiana.

A three-level testing process is utilized. Level I utilizes analytical solutions to debug codes and verify that the mathematical solutions are accurate. Level II testing incorporates further theoretical problems and results of laboratory tests and examines model responses to density differences, irregular boundaries, heterogeneities and anisotropies. Level III testing involves model calibration or history matching, using field data. Level III testing also utilizes the results of other codes in testing the code of interest.

In terms of discussion herein our procedure involves only two steps; Van der Heijde's Levels I and II as a first step, and his Level III as a second step. As an example of a classic problem with an analytical solution we illustrate the well known Theis well test problem.

WELL TEST PROBLEM

Consider the system shown schematically in Figure 16, a single production well in an infinite, single-phase slightly compressible fluid. The reservoir is homogeneous and isotropic (no directional properties) so porosity (ϕ), viscosity (μ), permeability (k), and compressibility (C_t), are constant. The well is producing at a constant rate, q, Bbls/day.

The pressure behavior at any point is:

$$p_i - p(t,r) = \Delta p(t,r) = 141.2 \frac{qB\mu}{kh} \quad p_D(t_D, r_D) + s$$

where;

$$t_D = \frac{0.0002637kt}{\phi\mu C_t r_w^2} \quad \text{and} \quad r_D = r/r_w$$

and;

q	=	flow rate, Bbls/D
B	=	formation volume factor, STB/RB
μ	=	viscosity, cp.
K	=	permeability, md.
h	=	formation thickness, ft.
pi	=	initial reservoir pressure, psi
p(t,r)	=	pressure at any future time, t, and distance, r, from the well of interest

Here, p_D is dimensionless pressure as defined by this equation, t_D is dimensionless time, and r_D is dimensionless radial distance. s is the "skin" at the wellbore, so-called since damage may result from drilling, causing additional pressure drop at the well which is not a reservoir property. Skin can, however, be negative for a hydraulically fractured well or wellbore improved by acidizing. The constant, 141.2, is necessary to render the equation consistent in oilfield units.

For a single well in an infinite-acting system P_D is given by the line source [Theis(1935)] solution if $r_D > 20$ and $t_D/r_D^2 > 0.5$ or if $t_D/r_D^2 > 25$.

$$p_D(t_D,r_D) = -\frac{1}{2} Ei\left[\frac{-r_D^2}{4\,t_D}\right]$$

where:

Ei(x) is the exponential integral

$$Ei(x) = -\int_x^{\infty} \frac{e^{-u}}{u}\,du$$

The values for this integral may be found in most mathematical handbooks Abramowitz and Stegun,(1965).

A simple well test problem can be utilized to see if the numerical simulator in question can produce an answer which is comparable to the Theis solution (see Figure 17). Figure 18 also illustrates the approximation of the Theis solution when $r_D = 20$. This work is the work of Mueller and Witherspoon(1965).

There are other problems with exact analytical solutions. Most documentation associated with numerical simulators contains example problems which include comparisons of analytic solutions. An example of this is the SWIFT II (and III) simulator. A self teaching guide, associated with SWIFT II documentation(1986), can be obtained which includes example problems with comparisons of numeric and analytic solutions. Analytical solutions must be chosen which test the intended purpose of the numerical code. Solutions to example problems appear in the Appendix.

DATA REQUIREMENTS

Data requirements for reservoir simulators can be divided into four broad categories: Geology, Rock Properties, Fluid Properties, and Historical Performance data. There are certain minimum requirements for each category of data which apply to all simulators. In addition, there are additional minimum requirements which apply only to certain problem and simulator types. Finally, there is a vast assortment of possible data which, though not required by the simulator, could be used to develop an understanding of the relevant reservoir mechanisms and greatly benefit the accuracy of the simulation results.

The following section of this report discusses methods of data development which should be useful to the reader. Underground reservoir systems can be sampled directly at bottomhole well penetrations, but if direct measurements are not available we must resort to indirect methods of measurement. If neither direct or indirect methods of measurement are possible, suggested methods of estimation for important parameters are given. To a great extent the accuracy of the final operable model depends on the diligence of the data development phase especially in the interpretation of the geological model.

REQUIRED DATA

Here we present a "shopping list" of required data without elaboration of where it comes from or how to judge its quality. In the following chapter we will address the sources and quality of data.

In an earlier chapter we discussed problem and simulator types and utilized as a major delineation, whether the injected fluid was aqueous or an immiscible solvent. Here we give data requirement lists separated into these same two groups. All data listed for the aqueous injectant are also required for the immiscible injectant. In addition the immiscible injectant requires data beyond that required of the aqueous injectant. Those additional data are listed in the immiscible column. The following table contains the data requirement list.

RESERVOIR SIMULATION DATA REQUIREMENTS

Category	Aqueous Injectant	Additional Data Required for Immiscible Injectant
Geology	Structure Map(s) Layer Thicknesses Areal Extent of Reservoir(s) Zonation(s)	
Rock Properties	Permeability } By Geologic Porosity } Layer Thickness	Saturation Map
	Compressibility Dispersion Coefficient (Dispersivity) Coefficient of Molecular Diffusion	
Fluid Properties	Compressibility	Relative Permeabilities
	Density Pressure Map (Potentiometric Surface)	
As function of pressure	Viscosity Formation Volume Factor	Solution Gas Ratio
Grid Data	Grid size - x, y, Layer thickness - z	
Well Data	Location in grid Perforated interval Injectivity (producing) coefficient	

SIMULATOR GRIDS

Examples of simulator grids are illustrated in Figures 1 through 4. Annotations with each grid explain possible applications. Each block or cell in a grid must have the certain data assigned before the model will compile or be initialized properly. Most simulators have a data checking routine which will not allow a model with incomplete data sets to be run. This feature reduces costs in disallowing execution with incomplete data sets.

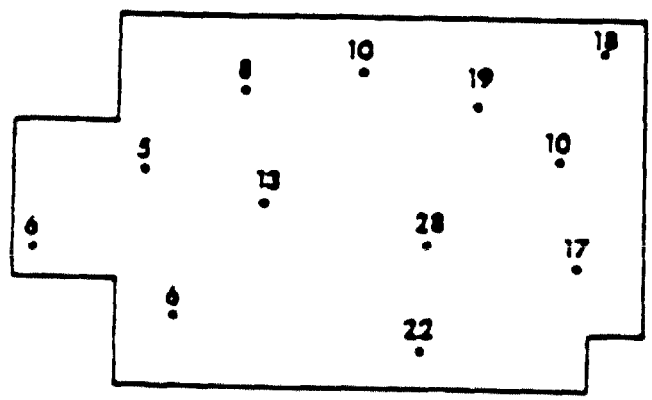
GRID DATA HANDLING

After the type of model has been selected, the reservoir is divided into a number of cells or blocks. Each cell is identified by its x-, y-, or z-coordinates or most often, by its i-, j-, k-indices. Normally, the reservoir is considered sealed on its exterior boundaries although efflux or influx at an assigned pressure or rate can be specified.

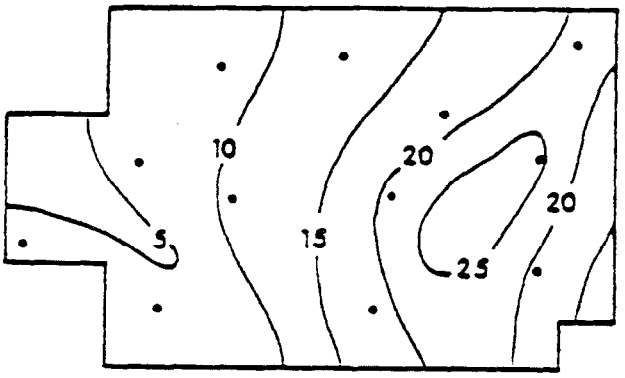
To each cell, we must assign the following: rock properties, geometrical data and well data (if the cell is a well block). The (specific) rock data are permeability and porosity. The geometrical data consist of the cell dimensions, i.e., Δx, Δy, and thickness Δz (or h), and the cell elevation relative to some datum. If a well falls in a block then pertinent well data must be included such as well type, rates, completion intervals, etc.

The values of permeability, porosity, bed thickness and subsea elevation must be assigned to each grid block or cell. This information is usually obtained from previously prepared contour maps. The actual data may come from cores, from well test results, or from downhole logs. The usual procedure is to overlay a transparency of the grid on such detailed maps and then read off the appropriate values and assign them to each grid block. This frequently will require interpolation between specified contour lines. In so doing, some error is introduced into the data that is assigned to each cell within the reservoir. Frequently it will be necessary to get averages of some of these values for each block. Since some of these data may be modified during the history matching stage, it is usually sufficient to do rather simple calculations to get these averages.

Data are generally available at well locations, however, data are needed for the total reservoir area. To obtain the data at intermediate points, the following procedure is used.



Collect all data pertaining to the parameter being considered. Plot these data by location on a plan map of the region as illustrated.



Contour these data points to obtain an overall areal distribution consistent with good engineering judgement and known geological trends in the area.

	2	3	5	9	10	13	16	17	18	18
	3	4	6	10	12	15	17	19	17	16
3	3	4	5	10	12	15	18	18	16	15	13
4	4	5	5	12	16	19	21	23	20	16	12
6	6	6	9	14	18	21	25	28	26	20	16
	6	8	13	16	18	23	24	22	19	17
	6	9	13	15	17	21	18	16	14	

Digitize the contoured data to obtain the required rock data values at intermediate points as shown.

BOUNDARY CONDITIONS

The mathematical rigor of specific boundary conditions will be addressed in Appendix I. Some pragmatism regarding their applications should be mentioned here.

Mercer and Faust(1980) have conveniently summarized the boundary conditions for groundwater problems. For steady-state problems only boundary conditions are required while for unsteady state problems both boundary (space) and initial conditions (time) are required. In physical terms, for groundwater applications the boundary conditions are generally of three types; (1) specified value, (2) specified flux or (3) value dependent flux, where the value is head concentration or

temperature, depending on the equation. The following table from Mercer and Faust(1980) gives additional description.

Ground-Water Boundary Conditions

Type	*Description*
Specified Value	Values of head, concentration or temperature are specified along the boundary (In mathematical terms, this is known as the *Dirichlet condition*.)
Specified Flux	Flow rate of water, concentration or temperature is specified along the boundary and equated to the normal derivative. For example, the volumetric flow rate per unit area for water in an isotropic media is given by $$q_n = -K\frac{\partial h}{\partial n}.$$ where the subscript n refers to the direction normal (perpendicular) to the boundary. A *no-flow (impermeable) boundary* is a special case of this type in which $q_n = 0$. (When the derivative is specified on the boundary, it is called a *Neumann condition*.)
Value-Dependent Flux	The flow rate is related to both the normal derivative and the value. For example, the volumetric flow rate per unit area of water is related to the normal derivative of head and head itself by $$-K\frac{\partial h}{\partial n} = q_n(h_b).$$ where q_n is some function that describes the boundary flow rate given the head at the boundary (h_b).

Initial conditions are values of head, concentration, or temperature inside the boundary at time t equals zero; i.e. p_i = constant (or a distribution based on structure). Normally an initial value(s) represents a system in equilibrium (heads calculated by structural elevation, etc.).

DATA DEVELOPMENT

The previous section of this manual discussed the data requirements for simulation problems. In this section, methods for developing various data are covered. The discussion is organized by data type under the categories of Geology, Rock Properties, Fluid Properties, and Historical Performance.

GEOLOGY

The selection of a geologic strata for waste disposal will be based on several criteria. The most important criterion is that of containment. Whatever the areal and vertical extent of the strata selected, we would like to know that the over-burden and under-burden should be of low enough effective permeability so that leakage will be within acceptable levels for whatever class of waste is being stored. Another criterion is that the strata selected be as far away as possible from any underground source of drinking water (USDW), and that the aqueous contents of the injection zone be unsuitable as a drinking water supply, i.e. greater than 10,000 TDS.

The result desired from reservoir modeling of underground storage of hazardous waste is a knowledge of the volumetric extent or "spread" of hazardous materials within an aquifer over time. The predicted spread of waste with advancing time will be very much affected by the geological properties assigned to the numerical model. The complexity of

subsurface geology should not be underestimated; we probably know less about sedimentologic properties and their vertical and spatial variations than any other variable within the model.

Since exploration and production of hydrocarbons has been a long standing economic activity in the world, we may investigate the role of geology in reservoir simulation studies through past experience in that industry. Harris(1975) has given an overview of the main features. Figure 19 illustrates the diversity and level of effort considered suitable in developing a proper geologic description of a hydrocarbon reservoir.

As discussed previously, the primary forms of geologic data required are information relative to the stratigraphy, sedimentology and structure of the rock within the area of interest. One cannot have too much geological data! Regional studies should be carefully reviewed. Examination of structure maps for faults should be noted as these may be open and provide conduits for leaks, or closed by mineralization and form barriers or partial barriers to flow. In order to make these determinations one must rely upon various methods. Regional geological studies will often provide insight into the depositional history of the proposed disposal area. In addition, analysis of transient pressure tests will sometimes indicate whether a known fault is open or closed to flow [Earlougher(1980)]. Regional earthquake activity should be considered for presence/absence of faults, seismic influences, etc. [van Poollen and Hoover(1970)]. Data from cores should be

accumulated and studied for rock and fluid properties (ϕ ,k, S_w, etc.). In short, every attempt should be made to understand the geology before constructing a numerical model. The geological information to be derived for the purposes of simulation consist of:

- zonation
- layer depths
- layer thicknesses
- structure
- stratigraphy

The following paragraphs discuss the data within each category, and the methods of measuring the data.

Zonation

The most important task in the geologic analyses is to determine the vertical zonation to be used in the simulation. Definition of the zonation requires a determination of the number of layers and of the boundaries of each layer. The number of layers selected will depend upon the nature of the rock, the location of barriers to vertical flow, and the information required from the simulation.

Frequently, the nature of the rock within the area of study allows for a natural zonation. Review of the logs and cores may suggest general layers which appear to have similar characteristics. Since individual

cells within the model will be assigned the average properties of the rock represented by that cell, it is undesirable for the cell to contain rock of widely varying characteristics. Model layers should be selected so that they represent a single rock type, rock with similar properties, or at least a set of strata whose degree of heterogeneity is similar.

The second criteria for zonation is the location of barriers to vertical flow. These barriers usually take the form of semi-permeable layers, such as shales or anhydrites. In most cases, the permeability of these barriers will be extremely low (0.000001 md to 0.01 md) when compared to the permeability of injection intervals. Borst(1983) has performed a detailed study of shale permeability and compared three methods for determining shale permeability values when data are sparse. Results from the three methods compare favorably. The equation requiring the least data is:

$$\text{Ln } [K] = C_1 + C_2 \, (A + C_3)^{C_4} B^{C_5}$$

where k in millidarcies and;

C_1 = -4.44,

C_2 = -0.822,

C_3 = 30.4,

C_4 = 0.085, and

C_5 = 0.266.

A is the geologic age of the sample in millions of years and B is the burial depth in meters. If the impermeable layer has negligible effective pore volume, it will most likely not be necessary to represent it as a model layer for a horizontal flow and transport problem. Reduced vertical permeability effects can be modeled as a reduction in interblock transmissibilities without requiring an additional physical layer. The barrier probably will not be totally sealing. Shales which are discontinuous, fractured, or faulted may be represented as some small, non-zero, value of permeability. The effect on vertical flow of discontinuous permeability barriers within model layers can be approximated by methods proposed by Begg and King(1985), Prats(1972), Haldersen and Lake(1982), and others. Generally speaking, these methods treat the permeability reduction as an increased tortuosity.

Aquitard permeability can also be determined by well testing. Figure 20 illustrates the mechanical requirements of the pressure testing scheme required. Earlougher(1980) discusses the technique which requires alternate sequences of injection and shut-in of the well where waste is injected through the tubing. Pressure pulses are received by the gauges above and below the aquitard and analyzed to yield the vertical permeability of the aquitard. An example of the results is shown in Figure 21. One can see that permeabilities lower than 0.01 md may be very difficult to determine from this method. For more specific details regarding the technique the reader is referred to Earlougher's publication(1980).

Aquitard permeabilities can also be determined from laboratory testing. Laboratory testing requires samples of the aquitard material be collected while coring the well. Sidewall cores are usually unacceptable since the imbedment of the percussion cap fractures the samples. Most commercial core laboratories have equipment capable of measuring low permeabilities. The analysis will, however, be expensive to perform.

The last criteria for selecting zonation of the strata for simulation is the information required from the study results. The proposed regulations specifically state that the simulation should attempt to demonstrate that injected fluids will not migrate upward out of the injection zone. Inherent in this statement is the requirement that the injection interval should be modeled as a separate layer from the overlying layers. Ideally, the injection interval should be modeled as several layers in order to accurately track the vertical migration of the injected fluid within this zone.

Layer Depths

Once the model zonation has been determined, certain data are required by the simulator for each layer. The first set of data required are the depths of each layer top. The depths are normally entered into the model as vertical distance from a datum, such as sea level. These depths can be determined at specific wells by correlation of marker beds on well logs or cores. In areas where no wells penetrate the

strata of interest, depths can be estimated from geophysical data, such as seismic surveys. In the absence of information to the contrary, smooth interpolation of depth between wells is often assumed. However, in areas of known faulting, this assumption can be very poor. Additional data may be required to support the assumption that faults are not present.

Layer Thicknesses

After determination of the depths of each layer top, the gross thicknesses of each layer must be defined. This data is usually derived from well logs or cores. If no intermediate layers are present, the thickness of a layer is the difference between the depths of the top of the layer and the top of the next layer. However, if strata exists between layers which are not represented as a model layer due to negligible effective porosities, the thicknesses may be less than this difference. The thickness of a layer can never be greater than the difference between the depths of the tops of the two adjacent layers. In areas where measurement is not possible, a smooth interpolation of thicknesses between wells is often assumed. This assumption can be checked against existing geophysical data. In areas of faulting or folding, this assumption may require support from additional data.

Structure

In any simulation study, a thorough analysis of structure should be made. Since direct structural data is generally only available at well locations (with the exception of seismic shot-hole data), geologic interpretations will usually require important assumptions. Structural relations within the area of study are important in that they effect layer depths, thicknesses, and flow of fluids. The first two items were discussed in previous sections. The primary elements of structure which effect fluid flow are faults and fractures (and folds, to some degree). These features can either speed or retard injected fluids depending on whether they are open conduits or sealed barriers. As these features can result in rapid penetration of seemingly impermeable confining layers, their identification is critical to the results of these studies. Faults and fractures often appear in areas of compressional deformation. However, it should be remembered that these features are also common in otherwise undisturbed areas due to tensional forces. The absence of folds in the rock is not evidence supporting the absence of faults and fractures.

Stratigraphy

In addition to the definition of zonation, stratigraphic analyses are important in determining flow behavior. Flow of fluids within subsurface strata is effected by changes in the nature of the rock and discontinuities in layering. Changes in rock characteristics will be

discussed in a later section of this manual. Stratigraphic discontinuities, often referred to as pinchouts, can have the same effect on fluid flow as totally or partially sealing faults. The existence of pinchouts should be determined (from stratigraphic correlation and seismic data), their location defined, and their effect on layer transmissibility estimated.

ROCK PROPERTIES

The petrophysical characteristics of each layer must be specified in the model. If possible, areal variations in these characteristics should be defined and ranges of accuracy for each parameter should be estimated. The typical data required by the simulator includes:

- net thickness, h
- porosity, ϕ
- permeability, k
- relative permeability, K_{ro}, K_{rw}, K_{rg}
- capillary pressure, P_c
- rock & fluid compressibilities, C_R, C_w, C_o
- fracture properties (spacing, K_f, ϕ_f)
- chemical reactions (ion exchange or adsorption isotherm)
- Storage, $S = \phi c_t h \left(\frac{\rho g}{g_c}\right)$, fraction
- Transmissivity, $T = \frac{kh}{\mu}\left(\frac{\rho g}{g_c}\right)$, gal(day/ft)
- Pressure, p, psia

- Diffusion, D_o, ft^2/D
- Dispersion, k_ℓ, k_t, ft^2/D

The relative permeability and capillary pressure relations required by the simulator can be greatly simplified (or omitted) when only a single aqueous phase is present in the area of interest. When the injected fluid is also in the form of an aqueous solution, the problem becomes one of tracking dissolved concentrations rather than distinct fluid phases. Relative permeabilities reduce to straight lines between endpoints and capillary pressure effects can be ignored.

Most of the data required to define the rock properties of each layer are derived from log, core, or pressure test analyses. The following sections describe the required data.

Net Thickness

Zones containing porous rock also often contain streaks of clay-filled, "dirty" rock (argillaceous material). Shaley streaks of a few inches of shale laminae which generally do not contribute to the storage or transport of fluids may be in evidence. By inclusion of this material, we refer to the porous reservoir interval as gross "pay" or gross thickness. When computing reservoir fluid flow capacity, kh in md ft, we are dealing with the net effective interval(s). It is important to differentiate between gross and net interval when constructing models and to assign porosities and permeabilities accordingly.

Porosity

The storage capacity, or $\phi c_t h$, is important since rocks with a large capacity will take longer to fill up thus retarding the spread outward. In general, sandstones in an intermediate depth range of 2000 to 5000 feet usually have an approximate porosity of 20 percent while those at 15,000 feet are often in the 8 to 10 percent range. This result occurs because at deeper horizons the compressive stresses from over-burden literally compact the sand grains, cements, and other argillaceous materials closer together leaving less pore space and less permeability. There is, of course, a considerable scatter of porosity and permeability from foot-to-foot in a core analysis. This scatter is due primarily to local depositional and post-depositional changes in rock fabric, i.e. amounts of clays, cements, silts, etc.

Permeability

Alpay(1972) describes a practical approach to defining reservoir heterogeneity. Figure 22 is from Alpay and illustrates the vertical heterogeneity in permeability over a twenty-five foot section in one well. It is this variation in horizontal permeability over the injection interval which is a prime variable in describing the "spread" of injected hazardous waste. Certain layers of high permeability within a geologic member will cause the horizontal spread of waste faster than others. The intercalations of clay and shale in sandstone systems act as baffles and retard the vertical movement

between sand members and reinforce the horizontal spread. If the example in Figure 22 were represented by an average horizontal permeability (k) the value would be well below 5 millidarcies for a total net thickness (h) of 25 feet. Individual members are between 3 and 23 millidarcies and each are only four or five feet thick; some thinner. Yet the total reservoir capacity, kh, in millidarcy feet, will be the same for each case. The spread of waste in the one layer case with an average kh would be severely underestimated when compared to a model with some individual layers having a much higher kh per layer and some having a lower kh per layer.

Porosity and permeability are variable in an areal sense as well as in the vertical sense. The shapes of reservoir bodies from a plan view may be extremely variable depending upon whether the reservoir is a stream deposited (fluvial) sand, a beach type deposit, or an offshore marine deposit. The amounts of argillaceous material may vary spatially causing corridors of high permeability which affect the spread of injected waste.

Relative Permeability

Relative permeability is that fraction (0.0-1.0) of absolute permeability of the rock which is available for flow to each phase at a specific phase saturation. Absolute permeabilities are usually determined from dry cores with air flow across the core. In general, the higher the phase saturation in the core the higher the relative perm-

eability accruing to that phase. Figure 9 illustrates oil-water and gas-liquid (water and oil) relative permeability curves. These curves are developed from laboratory coreflood data with carefully prepared core material.

Capillary Pressure

When a capillary tube is immersed into a liquid a rise of liquid into the tube is noted. Similarly, when a core plug is immersed liquid rises into the rock. It is this phenomena that causes the saturation interface between two phases to be smeared. The difference between oil phase pressure, p_o, and water phase pressure, p_w, is the capillary pressure, p_{cow}. Figure 10 illustrates the capillary pressure of an oil-water system.

Rock Compressibility

Rock compressibilities are generally on the order of 10^{-6} psi^{-1}. Compressibility is defined as:

$$C_R = \frac{-1}{V}\left(\frac{\partial V}{\partial P}\right)$$

so it is the change of volume with change in pressure divided by the volume. In a multiphase system the total compressibility, C_t, is:

$$C_t = C_R + S_o C_o + S_w C_w + S_g C_g$$

where S and C are the phase saturations and compressibilities for oil, water, and gas (so subscripted o, w, g).

Fracture Properties

Comments made to this point have dealt with single porosity/permeability systems; i.e. non-fractured systems. For fractured rocks, simulators must have the capability of containing fracture permeabilities and porosities as well. In addition, one must know the frequency of fracture occurrence in each of the three principal directions (x-y-z). Since fracture porosities are seldom greater than 2 or 3 percent, the storage capacities of fractured rocks are generally poor unless the associated rock matrix contains primary porosity as well. In addition, one must examine the reasons why fractured systems are fractured in the first place since the over-burden and under-burden rocks could be fractured as well thereby making confinement extremely questionable. Determination of the frequency of natural fractures and their permeability and porosity is difficult. In some cases these data can be derived from transient pressure testing; Gringarten(1984), and in some cases from reservoir formation test (RFT) data; Aguilera (1980).

Chemical Reactions

The kinetics of chemical reactions is so varied that a whole treatise could be written on the topic. Scrivner et al(1986) has given a

recent and succinct synopsis. A simplified list of characteristics for hazardous waste that was taken from Scrivner(1986) lists pH < 2 or pH > 12.5, cyanide ions > 1000 ppm or metal ions such as As > 5 ppm, Ba > 100 ppm, Cd > 1 ppm, Cr > 5 ppm, Pb > 5 ppm, Hg > 0.2 ppm, Se > 1 ppm, and Ag > 5 ppm.

Injected wastes are degraded or transformed by the following general processes; 1) neutralization, 2) hydrolysis, 3) coprecipitation, 4) ion exchange 5) microbial degradation, and 6) waste concentrating mechanisms. Neutralization reactions include carbonate, sand, and clay dissolution. Hydrolysis usually renders a material less hazardous; several examples are given -- hydrogen cyanide hydrolyzes to formamide which hydrolyzes to formic acid, acetonitrile hydrolyzes to acetamide and hence to acetic acid, etc. Coprecipitation reactions usually involve iron or barium compounds; ferric chloride is precipitated as ferric hydroxide. Ion exchange occurs with most clays; heavy metals such as nickel, lead, and chromium, are exchanged into the clay lattice and calcium and sodium are released. Microbes can aerobically or anaerobically transform many organics. These reactions are usually much faster than hydrolysis, although hydrolysis can be effective at certain pH levels.

Hydrolysis is just one of the many chemical and physical processes that reduce the concentrations of hazardous constituents in deep-well environments. Examples of other processes are radioactive decay and biotransformation. These processes and others can all be lumped

together and called decay processes, because they all result in the destruction of the constituent over time. One measure of the rate of decay is the half-life, which is defined as the time required for the original concentration to decrease by one half. Most simulators (numerical and analytical) quantify a transport species' half-life degradation through the use of an input parameter known as the decay constant. The decay constant (λ) of a species is related to the half-life (t 1/2), by the following equation:

$$\lambda = \ln 2/[t\ 1/2]$$

Petitioners who include any decay processes in their transport predictions will have to substantiate their chosen decay rate(s) with geochemical studies.

Although Scrivner et al(1986) doesn't specifically describe it, adsorption is also a mechanism which removes ions from injected solutions. An example of an adsorption isotherm is given in Figure 15. This example was taken from Shah and Schechter(1977), and is typical of petroleum sulfonate adsorption on Berea sandstones. This type of adsorption is thought to be physical and to some degree reversible. Adsorption is measured using carefully conducted coreflood experiments.

If an adsorption isotherm can be considered linear and the adsorption on the rock matrix reversible, then the isotherm can be described by the following equation:

$$\overline{C} = K_d C.$$

$\overline{C}$ equals the adsorbed concentration, C equals the solute concentration, and K_d is a constant which is called the distribution coefficient. Many numerical models use the distribution coefficient, along with the bulk density of the rock (p_b), and the effective porosity of the rock (ϕ), to describe adsorption of the solute on the rock matrix. However, many numerical and analytical models use a single parameter, the retardation factor (R), to describe adsorption. The retardation factor is defined by the following equation (Javandel, et al., 1984):

$$R = 1 + \left[\frac{p_b K_d}{\phi}\right]$$

The retardation factor can be described as the ratio of the average pore water velocity to the average solute velocity. Retardation factos can range from 1 to 1000, with one representing no retardation and 1000 is the estimated maximum value for retardation through shales (Morganwalp, 1988).

Hounslow (1983) has shown how to estimate the K_d of organic chemicals using octanol-water partition coefficients (K_{o-w}), and the total organic carbon content of the rock (%OC). The octanol-water partition is the partitioning of a solute between water and an immiscible organic solvent. This coefficient is a good measure of sorption and is the most commonly measured parameter in laboratory studies. The adsorp-

tion coefficient (K_{o-c}) is related to the octanol-water partition coefficient by the following equation,

$$K_{o-c} = A\ K_{o-w}$$

where A ranges between 0.4 and 0.6. The distribution coefficient is related to the adsorption coefficient by the following equation:

$$K_d = \frac{\%OC\ K_{o-c}}{100}$$

As with decay, petitioners who include any adsorption processes in their transport predictions will have to support their chosen adsorption isotherm(s) with geochemical studies.

SOURCES OF ROCK PROPERTY DATA

Logs

When a waste disposal well is drilled it will be logged openhole through the zone of interest before the completion is made. A spontaneous potential (SP) and a formation resistivity log should be run. The results of these two logs plus the resistivity of the aquifer water will allow the porosity to be estimated. Assuming the water saturation is 100 percent the porosity (ϕ) from Archie's equation is:

$$\phi = \left[\frac{a\ R_w}{R_T}\right]^{1/m}$$

For sandstones a = 1.13 and m = 1.73. For limestones a = 1.0, m = 2.0. R_W is the resistivity of the aquifer water (in ohms) and R_T is the resistivity across the core saturated with reservoir brine (in ohms). R_T can be extracted from the logging measurements; R_W must be obtained by laboratory measurement on a sample of the aquifer water. In lieu of this estimate for porosity, one must run a much more complicated suite of logs and calculate a and m from the data.

For shaly sands the calculation of porosity is best done by the Waxman-Smits(1968) method. The development of material for this subject is too detailed for presentation here; the reader is referred to the publication.

Well Tests

After the well is completed a constant rate injection test followed by a shut-in period should be performed. Prior to the injection period, a downhole pressure gauge run on a wireline should be placed at the mid-point of the perforations. This gauge can be equipped with a surface read-out or a mechanical clock. If the gauge has a mechanical clock, it should preferably have a 48 or 72 hour clock in case multiple injection/shut-in periods are required. A static pressure will be recorded once the gauge is on bottom. Once injection begins a pressure buildup will be recorded and following shut-in a pressure falloff will be recorded. If the gauge has a surface read-out, these pressure transients will be directly observable on a chart at the

surface. If a gauge with a mechanical clock is utilized, the gauge will be retrieved and the chart removed for reading.

Analysis of the pressure transient data will provide a formation capacity (kh). Division by the net thickness will yield an average permeability of the interval. If only a small portion of the total geological layer is perforated, a skin (wellbore damage) may be noted due to the spherical nature of flow near the perforations.

Spinner Survey

The perforated interval may include several sands in layers, and the distribution of permeability will not be determined by the transient test results. The permeability distribution about this average well test permeability needs to be determined because it is the sand members with greatest permeability that will be responsible for greatest and most rapid spread of the waste. If the permeability distribution is not developed, the model calculations for spreading of injected waste will be under estimated.

In order to obtain an estimate of the permeability distribution, a spinner survey should be run during an injection period. A spinner is a mechanical device run on a wireline that rotates in the passing flow stream like a propeller. The rotations are recorded and are proportional to the flow rate at the particular depth. The survey begins at the top most perforation and the rpms are recorded. The total flow is

passing through the spinner. The spinner is then lowered some increment downward, for example 10 ft. Now the rpm recording will be less if some flow is entering the formation above the spinner. From the difference between adjacent depth rpms, one can calculate the flow entering the formation over that depth increment. In this way, a distribution of flow over the complete perforated interval will be recorded. From the radial form of Darcy's law for steady-state flow, the permeability of each zone can be estimated.

Dykstra-Parsons Permeability Distribution

Craig(1971) gives a discussion regarding the coefficient of permeability variation (V_{DP}) as developed by Dykstra and Parsons(1950). If a spinner survey is not run, there will be no data regarding the vertical distribution of horizontal permeability. In an effort to provide a technique from which to estimate the distribution, it is suggested that the average permeability from the well test be utilized together with an estimate of V_{DP} to calculate a permeability distribution. The definition of V_{DP} is:

$$V_{DP} = \frac{\bar{k} - k_{\sigma}}{\bar{k}}$$

The value $\bar{k}$ is the mean permeability, that is, the permeability with 50 percent probability of occurring. The value k_{σ} is the permeability

at 84.1 percent of the cumulative sample. Most reservoirs have a V_{DP} between 0.6 - 0.85 with the more homogeneous at the lower value of V_{DP}. If $\bar{k}$ is known from a well test, and we assume a value for V_{DP}, we can calculate k_σ . A graphical presentation of V_{DP} vs. sample permeabilities is shown in Figure 23. Since the variation is a straight line on probability paper, we can graph our variation with two points, $\bar{k}$ at 50 percent and k_σ at 84.1 percent. From the distribution we can estimate the permeability variation to be used in the model.

FLUID PROPERTIES

The simulator requires characterization of both the in situ fluids and the injected fluids. It is expected that a single aqueous phase will exist in the area of interest before injection begins. The properties of this in situ water may vary areally or vertically depending upon the content of dissolved gas and solids, and variations in pressure.

The properties of the injected fluid will depend upon the fluid composition and changes in pressure. These properties should be defined at subsurface temperatures. Temperature effects on both the injected and in situ fluids can then be ignored. In addition if changes in fluid composition are small, for purposes of simulation, a constant injected fluid composition should be assumed. If there are large changes in injected fluid composition, then these can be accommodated by changes in the historical data specified for the simulator. The

properties of the combined fluids, in the case of miscibility, is a function of the relative proportions of the two fluids.

The primary properties required for the in situ and injected fluids are:

- viscosity
- density
- formation volume factor
- solution gas-oil ratio
- miscibility, dispersion and diffusion characteristics

These properties may be found in several references; Numbere et al(1977), Standing(1977).

The following section describes how these properties should be derived for each of the fluids of the simulation.

Viscosity

The viscosity of the fluid is given in centipoise. The viscosity is a function of pressure as shown in Figure 24. In reservoir fluid systems, as pressure is increased, the fluid will hold more gas in solution; eventually the fluid becomes saturated and will hold no more gas. At this point, called the bubble-point, a bubble of free gas will appear as a separate phase. This concept is quite important in

simulation of oil field systems; probably less important for aquifers since water will hold only a few cubic feet of gas in solution (up to 20 cubic feet at several thousand psi).

Density

This is the density of the fluid measured as pounds mass per cubic foot. The density is usually taken at standard conditions.

Formation Volume Factor

The formation volume factor is simply the ratio of volume of the fluid at reservoir conditions, fully swollen with gas, to the volume of fluid at surface conditions of temperature and pressure. The formation volume factor is a function of pressure. The surface conditions are usually standard conditions (i.e. 14.7 psia and 60°F). Figure 25 illustrates the data; the bubble-point is indicated BPT. The BPT is the pressure at which the first bubble of free gas emerges from the liquid.

Solution Gas-Oil Ratio

This is the amount of gas held in solution by the reservoir fluid, as a function of pressure. It is expressed as the volume at standard conditions (14.7 psia and 60°F) per reservoir volume of fluid (cubic feet or barrels). Figure 26 illustrates the functionality of R_s vs. pressure. The bubble-point is indicated.

Miscibility, Dispersion, and Diffusion

In miscible flow, where injectant and displaced aquifer water mix in all parts with no phase separation, diffusion and dispersion are often quite important in determining the spread of waste.

The diffusion coefficient, D_o, is a molecular property and for pure fluids is available in various handbooks. We refer to D_o as a fluid property. In small tubes, called capillary tubes, the diffusion coefficient is equal to the molecular fluid property D_o since all cross-sectional area is open to flow. Capillary tube models are not representative of flow in porous media since in porous media fluid flow paths are longer due to flow around sand grains. In fact flow in porous media moves at a mean direction of about 45° to the average direction of flow so the effective diffusion in porous media, D_e, is approximately equal to $1/\sqrt{2}$ or $0.707\ D_o$. A number of investigators have recognized that there is an analogy between diffusion and electrical conductivity in porous media since the current and flow paths are the same. The relationship between molecular diffusion, effective diffusion and electrical resistivity in porous media is:

$$\frac{D_e}{D_o} = \frac{1}{F\phi}$$

where:

D_e = the effective diffusion coefficient in porous media, ft^2/d

D_o = the molecular diffusion coefficient, ft^2/d

F = formation electrical resistivity factor

ϕ = fractional porosity

According to Wyllie and Spangler(1952) a further relationship exists. The complex flow paths in porous media are often referred to as tortuous. The average length of all flow pathways divided by the length of the core is called the tortuosity, τ, and $\tau = F\phi$ so the previous equation for effective diffusion in porous media can be restated as;

$$\frac{D_e}{D_o} = \frac{1}{\tau}$$

Values for τ range between 1.4 and 2.0. Frick(1962) provides a general synopsis for this subject.

Dispersion, often called hydrodynamic dispersion, is caused by mechanical mixing of the injectant and in situ water in the different length pore pathways. The amount of dispersion to be expected is a function of the velocity of flow and the rock geometry. An early paper by Perkins and Johnston(1963) presents the fundamental relationships of diffusion and dispersion in porous media in a reasonable and understandable fashion. Dispersion and diffusion in unconsolidated porous media are related as follows;

$$\frac{K\rho}{D_o} = \frac{1}{F\phi} + 1.75\,\frac{Ud_p}{D_o}\,; \qquad \frac{Ud_p}{D_o} < 50$$

where:

K_ℓ = longitudinal dispersion, ft^2/day

U = interstitial velocity, v/ϕ , ft/day

d_p = average particle diameter, ft.

Units can be in any consistent set so as to render the groups K_ℓ/D_o and Ud_p/D_o dimensionless. The group, Ud_p/D_o is often called a Peclet number because it is the ratio of convective movement due to velocity divided by the movement due to diffusion which is caused by concentration gradients.

The proportionality constant 1.75 may change depending upon the type rock, and whether we are examining laboratory coreflood results or tracers from field tests. The importance of the equation is that it describes dispersion as a sum of diffusion and velocity/rock geometry factors. When velocities are low, effective diffusion ($D_o/F\phi$ or D_e) controls the value of K_ℓ . When velocities are high, D_e becomes insignificant compared to 1.75 Udp, and K_ℓ is determined by the second term. Figure 27 illustrates the relationship of K_ℓ/D_o vs. Ud_p/D_o for unconsolidated porosity media, and shows the various regimes where diffusion controls and where convection controls.

Further comparison of dispersion with mixing cell theory is discussed by Perkins and Johnston(1963). An inhomogeneity factor, σ , is introduced which represents the randomness of packing in porous beds of beads. The equation for longitudinal dispersion is now:

$$\frac{K_\ell}{D_o} = \frac{1}{F\phi} + 0.5\,\frac{U\sigma\, d_p}{D_o};\quad \frac{U\sigma\, d_p}{D_o} < 50$$

This relationship is shown in Figure 28.

Dispersion and diffusion also occur in the direction orthogonal to the principal direction of flow. This dispersion is called transverse dispersion. The value for K_t is normally 10 to 30 times smaller than K_ℓ. Perkins and Johnston(1963) give the relationship as;

$$\frac{K_t}{D_o} = \frac{1}{F\phi} + 0.055\,\frac{Ud_p}{D_o}$$

This relationship is shown in Figure 29. Values of σd_p are given in the following table from Perkins and Johnston(1963).

Values of (σd_p) for Outcrop Sandstones

Source	Dispersion	Rock	σd_p (cm)
Grane and Gardner,(1961)	Transverse	Berea	0.25
Brigham, et al(1961)	Longitudinal	Berea	0.39
	Longitudinal	Torpedo	0.17
Raimondi, et al(1959)	Longitudinal	Berea	0.46
Handy	Longitudinal	Boise	0.55
		Average	0.36

Other researchers, engineers, and hydrologists refer to the coefficient of velocity in the foregoing discussion as the dispersivity, α ft. The general forms of these relationships for longitudinal and traverse dispersion become;

$$K_\ell = D_e + \alpha_L U \quad \text{and}$$

$$K_t = D_e + \alpha_t U$$

where:

$$D_e = \frac{D_o}{F\phi} = \frac{D_o}{\tau}$$

These forms are now universally recognized. The values of α range anywhere from a few hundredths of a foot for laboratory investigations to several tens of meters for field work. Freeze and Cherry(1979) and Gillham and Cherry(1982) give a range of 1 x 10^{-5} cm^2/sec to 1 x 10^{-6} cm^2/sec for effective molecular diffusion coefficients in clay rich unconsolidated deposits. Ranges of field measured (or estimated) dispersivities are given in the following two tables from Anderson (1979).

Dispersivity of the Alluvial Aquifer at Chalk River, Ontario[9]

Method	Dispersivity (m)	
	Full aquifer	Plane of high velocity
Single-well test	0.034	0.034—0.1
Two-well test	0.5	0.1

Dispersivity of the Alluvial Aquifer at Several Sites at Lyons, France[11]

Method	Mean velocity (m/day)	Longitudinal dispersivity (m)	Transverse dispersivity (m)
Single-well test	—	0.10—0.50	—
		stratum scale	—
		5.0 full aquifer	
Single-well test with resistivity	7.2	12.0	3.110—14.000
	9.6	8.0	0.0150—1.000
	13.0	5.0	0.145—14.500
	9.0	7.0	0.009—1.000
Environmental tracer		12.0	4.0

Dispersivities from Two-Well Tests

Type of aquifer	Location	Distance between wells (m)	Porosity	Dispersivity (m)	Ref.
Fractured dolomite	Carlsbad, N.M.	38.1—54.9*	0.12	38.1	152, 37
Fractured schist and gneiss	Savannah River Plant, S.C.	538	0.0008	134.1	159, 37
Alluvial sediments	Barstow, Calif.	6.4	0.40	15.2	34
Alluvial sediments	Tucson, Ariz.	79.2	0.38	15.2	cited by Robson[34]
Fractured chalk	Dorset, England	8	0.005	3.1	161
Chalk	DORSET, England	8	0.023	1.0	161

* Inclined hole; 38.1 m at surface.

Regional Dispersivities (m)

Type of aquifer	Location	Porosity	Longitudinal dispersivity (m)	a_t/a_l	Nodal spacing (m)	Type of model	Ref
Alluvial sediments	Rocky Mountain Arsenal, Col.	0.30	30.5	1.0	305	Areal	29
	Colorado	0.20	30.5	0.3	660 × 1320	Areal	30
	California	NR	30.5	0.3	305	Areal	32
	Lyons, France	0.2	12	0.33	NR	Areal	21
	Barstow, Calif.	0.40	61	0.3	305	Areal	34
	Sutter Basin, Calif.	0.05—0.2	80—200	0.1	Variable	3-D	136
Glacial deposits	Long Island, N.Y.	0.35	21.3	0.2	Variable	Areal	74
Limestone	Brunswick, Ga.	0.35	61	0.3	Variable	Areal	16
Fractured basalt	Idaho	0.10	91	1.5	640	Areal	33
		0.10	91	1.0	640	Areal	48
	Hanford site, Washington	NR	30.5	0.6	NR	Areal	50
Alluvial sediments	Barstow, Calif.	0.40	61	1/330	3 × 152	Profile	35
	Alsace, France	NR	15	0.067	NR	Profile	21
Glacial till over shale	Alberta, Canada	0.001 and 0.053	3.0 and 6.1	0.2	Δ_x = 79	Profile	36
Limestone	Cutler area, Fla.	0.25	6.7	0.1	Variable	Profile	121
	Hypothetical	0.10	0.003—30	0.2	Δ_x = 30.5	Profile	110
		0.3	21.3	0.2	Variable	profile	45
		0.02—0.2	10.	—	NR	1-D	113
		0.3	0.5—100	1—0.05	12.5 × 25	Profile	88

Note: a_l = longitudinal dispersivity; a_t = transverse dispersivity; NR = not reported; 3-D = three-dimensional, 1-D = one dimensional, areal and profile refer to two-dimensional models.

In applying large values of dispersivity, i.e. macro-dispersivity, one must use extreme care. In many cases large values of dispersivity are utilized in simplified one-dimensional models instead of constructing a proper two- or three-dimensional model with proper geologic layers. In an attempt to rectify the lack of vertical heterogeneity in the one-dimensional model, the model is assigned a large dispersivity to spread the waste front when in fact the spread is caused by the more fundamental heterogeneity of layering. Inappropriate application of large dispersivities in a one-dimensional model will not correct the failure to understand and model the proper geological considerations of layering.

HISTORICAL PERFORMANCE

The last category of data required by the simulator involves measurements of the historical behavior of the wells and the reservoir. If injection has not yet begun, the only data required are estimates of initial pressures at the injection well(s) and of natural pressure gradients existing within the area of study. These estimates of gradients are very important in that movement of injected fluids over the 10,000 year period may be controlled by natural flow within the strata, rather than by pressure gradients imposed during the relatively short injection period.

If injection has taken place in the area of study, the required measurements of historical behavior include:

- injection rates/cumulatives
- flowing/static pressures at the injection wells
- pressures/concentrations at the monitor wells

This data will be used in the history matching process which is discussed in a later section of this manual. In this process, the model description is calibrated using measurements of reservoir response to injection. Reservoir behavior calculated by the simulator is compared to the actual field measurements. The reservoir description is adjusted until a satisfactory match is obtained. The injection rates are specified, and pressures and fluid compositions are the principle match parameters. The quality of the final reservoir description depends upon the quality of the initial description, as derived from geologic, petrophysical and fluid analyses, and on the quality and quantity of the historical performance data.

It is expected that in most cases, little or no historical performance data will be available. In situations where no information of this type is available, the quality of the model description will depend entirely on the initial data analyses phases. These analyses and estimations should be performed with great care, as no calibration will be possible. The implication of each assumption should be clear and sensitivity analyses should be performed to quantify the effects of uncertainties on the final results. Sensitivity analyses are discussed in a later section of this manual.

MODEL CONSTRUCTION

The previous sections of this manual have described the geologic and engineering analyses required prior to constructing the initial simulation model. The resulting reservoir description is by necessity, derived from measurements made at widely spaced points in the reservoir penetrated by wells. For the most part, these measurements do not reveal information about the reservoir far beyond the wellbore. Due to the small percentage of the reservoir directly sampled, and to the degree of inaccuracy of some of the measurements themselves, the initial reservoir description is approximate, at best. However, it is exceedingly important to derive the best reservoir description possible from the available data. This is underscored by the fact that little, if any, historical performance data is typically available for hazardous waste injection sites. This means that verification of the reservoir description from historical data will be difficult.

The quality of the reservoir description, and hence of the simulation results, will often depend more upon the assumptions made in constructing the model, than on the actual analysis of the data. This is a reflection of the fact that the quantity of data required by the model is often much greater than the data that has been actually measured in the field. It is therefore important that each assumption be made carefully and be stated in the text of the application. Certain assumptions may appear to be the most obvious but can still result in poor simulation results if incorrect. An example is the common

technique of constructing smooth contour lines on structure maps, based on a few data points. The assumption inherent in this technique is that the structural depths change smoothly between wells. Smooth structural changes between wells suggest that no major faults are present. Since faults can greatly alter the flow pattern of the injected materials, the basic assumption has significant consequences and should be considered with care.

The following section discusses numerical dispersion, overshoot, and model stability. Requirements for stability are discussed, and quantified values for numerical dispersion are given.

Grid Dimensions and Time Step Size

The problems associated with grid dimensions and time step size when solving the diffusion-convection (advection) equation are complex. Improper choices of spatial increment (Δx) and time increment (Δt) can cause dispersion larger than the physical dispersion desired, and/or unstable solutions which will not converge. It is the purpose of this section to explore this aberrant behavior and determine when it is likely to occur. The discussion here is based heavily on excerpted material from Peaceman(1977) and Lantz(1971).

We will first visit Lantz(1971) to acquire a "feel" for the finite difference approach, then we will visit Peaceman(1977) for some examples.

The convective-diffusion equation is:

$$\frac{\partial C}{\partial \tau} = D \frac{\partial^2 C}{\partial \xi^2} - \frac{\partial C}{\partial \xi} \qquad (1)$$

where:

$\Delta\tau$ is a dimensionless time variable expressed in pore volume, $\frac{vt}{\phi L}$

is a dimensionless distance variable, $\frac{x}{L}$

C is concentration, volume fraction (C/C_o)

D is dimensionless diffusivity, $D\phi/Lv$)

ϕ = porosity, fraction

v = Darcy velocity, ft/d

t = time variable, days

x = length variable, ft.

L = overall length, ft.

The first term on the right-hand side of the equation is the diffusion (dispersion) term, and the second term is the convective (velocity driven) term.

Difference Forms

An explicit expression for the truncation error (the space derivatives are approximated at a known time level) can be developed from a Taylor Series expansion.

$$\frac{C_{\xi,\tau+\Delta\tau} - C_{\xi,\tau}}{\Delta\tau} = \frac{\partial C}{\partial\tau}(\xi,\tau) + \frac{\Delta\tau}{2}\frac{\partial^2 C}{\Delta\tau^2}(\xi,\tau) + \frac{\Delta\tau}{6}\frac{\partial^3 C}{\Delta\tau^3}(\xi,\tau) + \ldots. \quad (2)$$

A similar expression can be written for a non-centered space derivative as:

$$\frac{C_{\xi,\tau} - C_{\xi-\Delta\xi,\tau}}{\Delta\xi} = \frac{\partial C}{\partial\xi}(\xi,\tau) - \frac{\Delta\xi}{2}\frac{\partial^2 C}{\partial\xi^2}(\xi,\tau) + \frac{(\Delta\xi)^2}{6}\frac{\partial^3 C}{\partial\xi^3}(\xi,\tau) \pm \ldots. \quad (3)$$

The approximation to the second-order space derivative is:

$$\Delta_\xi^2 C = \frac{C_{\xi+\Delta\xi,\tau} - 2C_{\xi,\tau} + C_{\xi-\Delta\xi,\tau}}{(\Delta\xi)^2} = \frac{\partial^2 C}{\partial\xi^2}(\xi,\tau) + \frac{(\Delta\xi)^2}{12}\frac{\partial^4 C}{\partial\xi^4}(\xi,\tau) + \ldots. \quad (4)$$

The finite difference approximation to the differential equation using a backward difference (BD) approximation to the space derivative is;

$$\frac{C_{\xi,\,\tau+\Delta\tau} - C_{\xi,\tau}}{\Delta\tau} = D\Delta_{\xi}^{2}C - \frac{C_{\xi,\tau} - C_{\xi-\Delta\xi,\,\tau}}{\Delta\xi} \qquad (5)$$

The corresponding differential equation being solved by this finite difference approximation, retaining only through second-order differentials is;

$$\frac{\partial C}{\partial\tau} + \frac{\Delta\tau}{2}\frac{\partial^2 C}{\partial\tau^2} = D\frac{\partial^2 C}{\partial\xi^2} - \frac{\partial C}{\partial\xi} + \frac{\Delta\xi}{2}\frac{\partial^2 C}{\partial\xi^2} \qquad (6)$$

From this equation it is apparent that an additional term with $\Delta\tau/2$ has been introduced. In addition a second order time-derivative truncation term has been introduced. Since the order of differentiation is immaterial we can differentiate the original equation with respect to time and also with respect to space and equate the two expressions. Performing these differentiations yields;

$$\frac{\partial^2 C}{\partial\tau^2}(\xi,\tau) = \frac{\partial^2 C}{\partial\xi^2}(\xi,\tau) - D\left(\frac{\partial^3 C}{\partial\xi^3}(\xi,\tau) + \frac{\partial}{\partial\tau}\frac{\partial^2 C}{\partial\xi^2}(\xi,\tau)\right) + \ldots. \qquad (7)$$

Substituting for the term $\partial^2 C/\partial\tau^2\ (\xi,\tau)$ in Eqn. (6) from Eqn. (7) yields the final equation,

$$\frac{\partial C}{\partial\tau}(\xi,\tau) = \frac{-\partial C}{\partial\xi}(\xi,\tau) + \left(D + \frac{\Delta\xi - \Delta\tau}{2}\right)\frac{\partial^2 C}{\partial\xi^2}(\xi,\tau) + \ldots \qquad (8)$$

Eqn. (8) is the partial differential equation being solved by the BD finite difference representation, Eqn (5). We now see that, due to

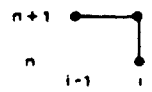
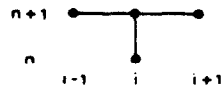
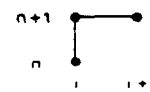
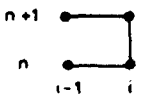
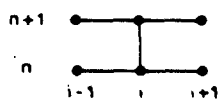
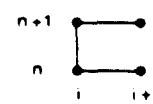
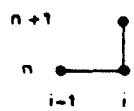
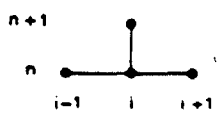
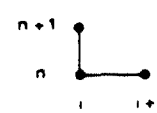
truncation error, the total dispersion in Eqn. (8) is $D + \frac{\Delta\xi - \Delta\tau}{2}$. The term $\frac{\Delta\xi - \Delta\tau}{2}$ is referred to as the numerical dispersion, while D is the physical dispersion.

As used here, both D and $\frac{\Delta\xi - \Delta\tau}{2}$ are dimensionless. If the dimensionless time step $\Delta\tau$, in pore volumes is equal to the dimensionless space increment, $\Delta\xi$, then numerical dispersion is zero for a backward difference space derivative and a centered in time second derivative. Due to excessive numbers of grid blocks this approach to reducing the numerical dispersion to zero is not always practical.

A similar development for a centered approximation to the first order space derivative yields a numerical dispersion that is negative, dependent on only dimensionless time step size, and equal to $\frac{-\Delta\tau}{2}$.

In addition to numerical dispersion the solution to the finite difference analogs of the convective-dispersive equation will become unstable under certain conditions; i.e. when numerical dispersion is negative. In all cases where the numerical dispersion is positive the finite difference solution is stable. Peaceman(1977) illustrates the full gamut of cases for distance and time differencing. A table from his book is reprinted here. For our purposes consider $f' = 1$. and $\lambda = \left(\frac{v\,\Delta\tau}{\Delta x}\right)$.

Special cases of first-order difference equation

	Backward-in-distance $W = 1$	**Centered-in-distance** $W = \frac{1}{2}$	**Forward-in-distance** $W = 0$
Backward-in-time $\theta = 1$			
	always stable $\mathfrak{D}_{num} = \frac{1}{2}vf'\Delta x(\lambda + 1)$	**always stable** $\mathfrak{D}_{num} = \frac{1}{2}vf'\Delta x(\lambda)$	**stable if** $\lambda \geq 1$ $\mathfrak{D}_{num} = \frac{1}{2}vf'\Delta x(\lambda - 1)$
Centered-in-time $\theta = \frac{1}{2}$			
	always stable $\mathfrak{D}_{num} = \frac{1}{2}vf'\Delta x$	**neutrally stable** $\mathfrak{D}_{num} = 0$	**always unstable** $\mathfrak{D}_{num} = -\frac{1}{2}vf'\Delta x$
Forward-in-time $\theta = 0$			
	stable if $\lambda \leq 1$ $\mathfrak{D}_{num} = \frac{1}{2}vf'\Delta x(1 - \lambda)$	**always unstable** $\mathfrak{D}_{num} = -\frac{1}{2}vf'\Delta x(\lambda)$	**always unstable** $\mathfrak{D}_{num} = -\frac{1}{2}vf'\Delta x(\lambda + 1)$

after Peaceman(1977)

Following further in Peaceman's footsteps we shall examine the behavior of several solutions of Eqn. (1). Remember that for

upstream space weighting, w = 1

mid-point space weighting, w = 1/2

downstream space weighting, w = 0

or:

$$C_{i+1/2} = (W)\, C_i + (1\text{-}W)\, C_{i+1}$$

and;

$$C_{i-1/2} = (W)\, C_{i-1} + (1\text{-}W)\, C_i$$

Time weighting is similar and designated by

implicit : $\theta = 1$

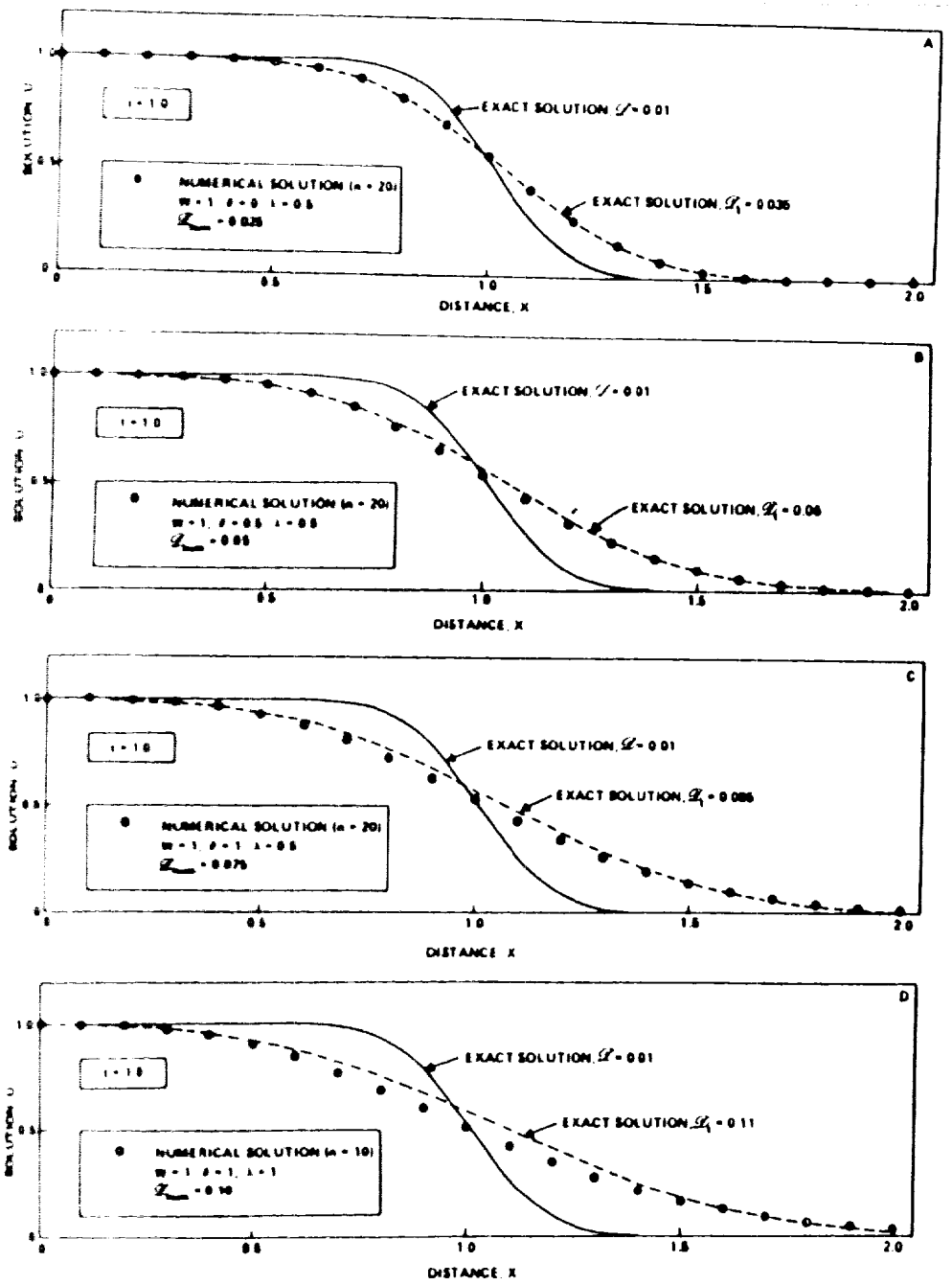
centered in time : $\theta = 1/2$

explicit : $\theta = 0$

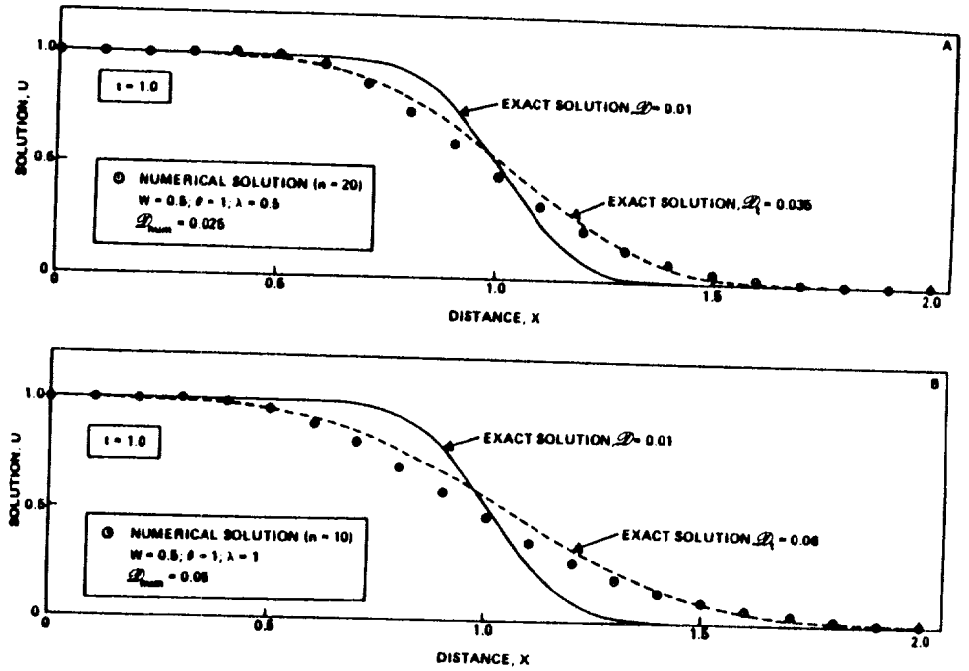
With these formalisms in mind we examine several figures from Peaceman.(1977) (Here the number of grid blocks are designated by "n".)

The following six figures show examples of solutions that exhibit significant numerical dispersion. In each case the exact solution to the analytical equation (the error function solution) for D = 0.01 and t = 1.0 is graphed as the solid curve. The numerical dispersion, D_{num}, is shown in the box in each figure. The exact analytical solution for $D_t = D + D_{num}$ is shown in each figure as a broken curve. Note that as D_{num} becomes greater due to unfavorable time and space increments the numerical solution becomes worse and worse as compared

to the exact solution for D = 0.01. The analytical solution represented by the broken curve remains fairly true in all cases.



Numerical solutions (of diffusion-convection equation) exhibiting numerical dispersion. Difference equations are backward-in-distance and: A. Forward-in-time, with $\lambda = \frac{1}{2}$. B. Centered-in-time, with $\lambda = \frac{1}{2}$. C. Backward-in-time, with $\lambda = \frac{1}{2}$. D. Backward-in-time, with $\lambda = 1$.

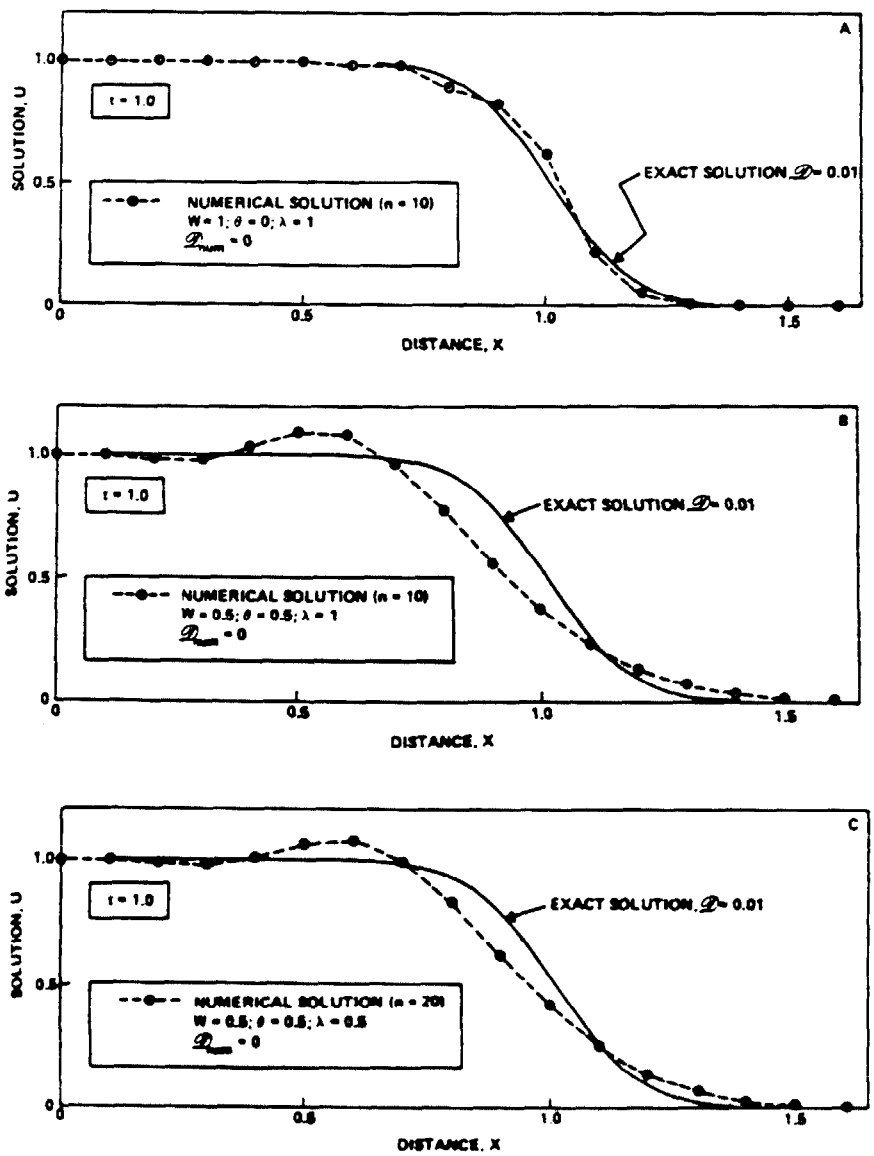


Numerical solutions (of diffusion-convection equation) exhibiting numerical dispersion. Difference equations are centered-in-distance and backward-in-time. A. $\lambda = \frac{1}{2}$. B. $\lambda = 1$.

after Peaceman(1977)

The next figure shows solutions for three cases where $D_{num} = 0.0$. Case A involves the backward-in-distance, forward-in-time difference equation for which zero numerical dispersion can be obtained only by choosing the time step, Δt, so that $\lambda = 1$. Excellent agreement is obtained, however the applicability of this approach is relegated to 1-D problems since in 2- or 3-D one cannot simultaneously control v_y and v_z to insure $\lambda = 1.$ in all three directions at once.

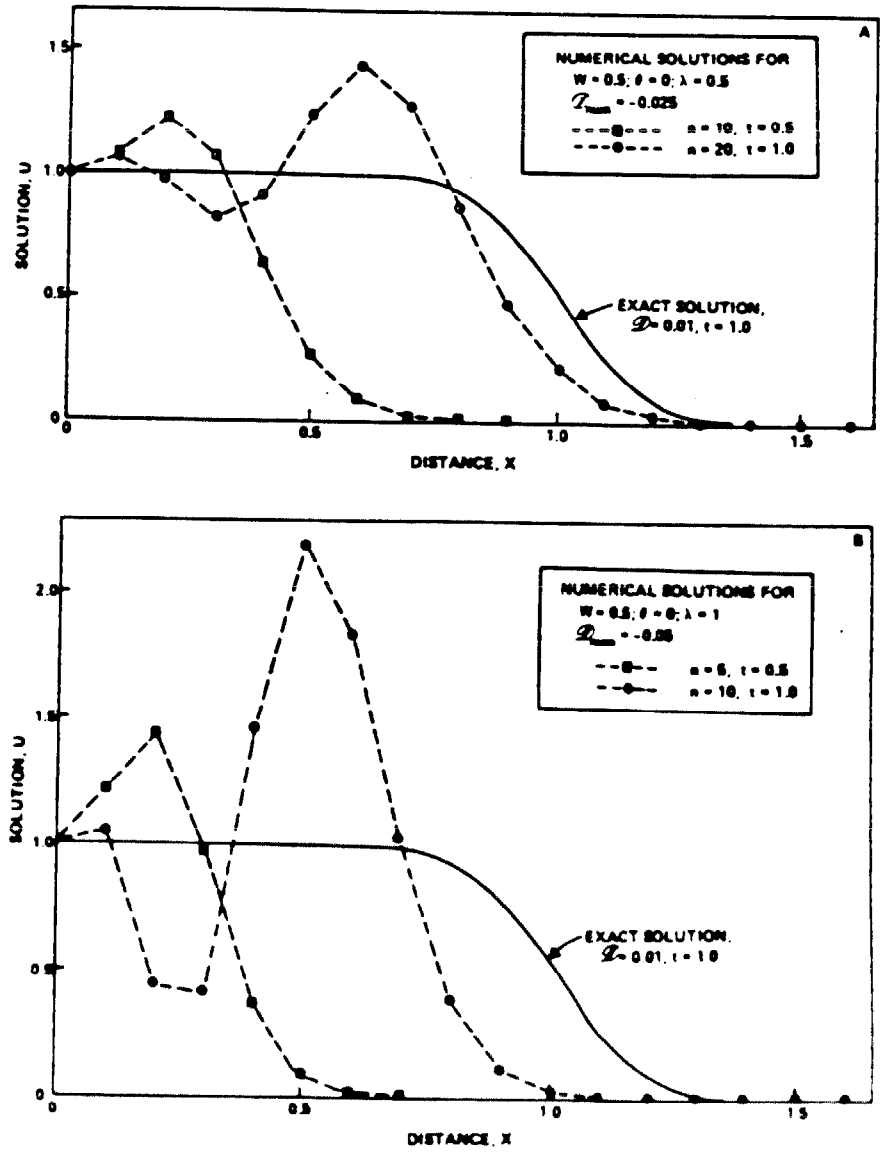
Cases B and C involve application of the use of centered-in-time and centered-in-distance difference equation. Here the solutions oscillate, a typical manifestation of higher order difference equations designed to eliminate numerical dispersion. In this the over-shoot becomes worse as the front becomes sharper (i.e. as the physical dispersion becomes smaller).



Numerical solutions (of diffusion-convection equation) with zero numerical dispersion. Difference equations are: A. Backward-in-distance, forward-in-time, with $\lambda = 1$. B. Centered-in-distance, centered-in-time, with $\lambda = 1$. C. Centered-in-distance, centered-in-time, with $\lambda = \frac{1}{2}$.

after Peaceman(1977)

The last figure shows two examples of unstable numerical solutions. These solutions were obtained with a centered-in-distance, forward-in-time difference equation. The total dispersion coefficient, $D_t = D + D_{num}$, is negative and the degree of instability, i.e. growth of oscillation per time step, grows as λ and $-D_{num}$ increase.



Numerical solutions (of diffusion-convection equation) exhibiting instability. Difference equations are centered-in-distance, forward-in-time. A. $\lambda = \frac{1}{2}$ B. $\lambda = 1$

Finally, Lantz(1971) provides some quantification of numerical dispersion as well. The following two tables illustrate both the error forms and observed and calculated numerical dispersion for various difference formulations for both miscible and immiscible problems. We are interested here only in the miscible problem.

The last figure illustrates ranges of diffusivity, $D\phi/vL$, where space increments are important. We are interested in miscible liquids, shown as the range $10^{-5} < D\phi/vL < 10^{-3}$.

TABLE 1 — SUMMARY OF TRUNCATION-ERROR EXPRESSIONS

Difference Form		Error Forms	
Spatial	Time	Miscible	Immiscible
BD	Explicit	$(\Delta\xi-\Delta\tau)/2$	$\frac{df_w}{dS_w}(\Delta\xi-\frac{df_w}{dS_w}\Delta\tau)/2$
CD	Explicit	$-\Delta\tau/2$	$-\left(\frac{df_w}{dS_w}\right)^2\Delta\tau/2$
BD	Implicit	$(\Delta\xi+\Delta\tau)/2$	$\frac{df_w}{dS_w}(\Delta\xi+\frac{df_w}{dS_w}\Delta\tau)/2$
CD	Implicit	$\Delta\tau/2$	$\left(\frac{df_w}{dS_w}\right)^2\Delta\tau/2$

TABLE 2—COMPARISON OF OBSERVED AND CALCULATED NUMERICAL DIFFUSIVITIES FOR VARIOUS DIFFERENCE FORMULATIONS OF MISCIBLE EQUATION

$\Delta\xi$	$\Delta\tau$	Calculated Numerical Diffusivity	D_{input}	D_{total}	Observed Numerical Diffusivity
		Explicit-Backward Difference			
0.01	0.0038	0.0031	0.005	0.0078	0.0028
0.01	0.002	0.0040	0.005	0.0088	0.0038
0.01	0.0005	0.00475	0.005	0.0096	0.0046
0.02	0.005	0.0075	0.001	0.0085	0.0075
0.02	0.005	0.0075	0.01	0.172	0.0072
0.02	0.02	0	0	0	0
		Explicit-Central Difference			
0.02	0.005	-0.0025	0.0125	0.0099	-0.0026
0.02	0.01	-0.005	0.015	0.0096	-0.0054
0.04	0.01	-0.005	0.015	0.0105	-0.0045
		Implicit-Backward Difference			
0.01	0.002	0.006	0.00005	0.0061	0.00605
0.01	0.0002	0.0051	0	0.0051	0.0051
0.01	0.01	0.01	0	0.0101	0.0101
		Implicit-Central Difference			
0.02	0.005	0.0025	0.0075	0.0101	0.0026
0.02	0.01	0.005	0.005	0.0101	0.0051
0.04	0.01	0.005	0.005	0.0107	0.0057

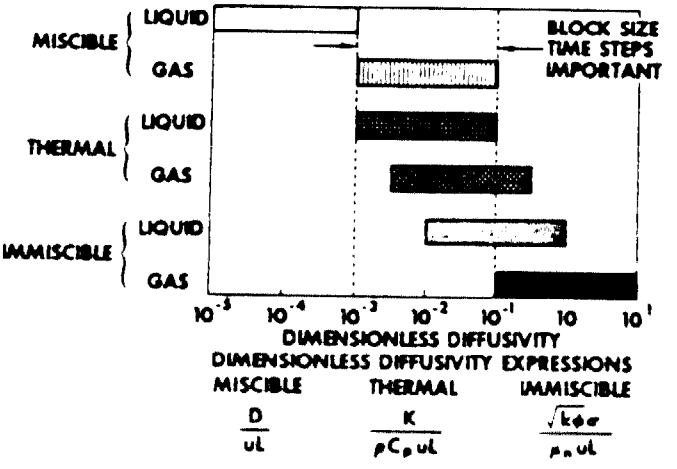


FIG. 2 — TYPICAL PHYSICAL DIFFUSIVITIES FOR MISCIBLE, THERMAL, AND IMMISCIBLE CASES.

after Lantz(1971)

Practical Considerations

With all the foregoing in mind, one method to use in sizing cells is to run a linear (horizontal strip) model with a total distance of several hundred feet in length. Divide the strip into 10 equal cells with $\Delta x = \Delta y$ and all with the same Δz. This strip will have an injection well in cell 1 and a production well in cell n. Inject waste at a rate commensurate with actual conditions. At the production well, graph C/C_o vs. time. Repeat the experiment with double the number of cells (i.e. half Δx). Regraph results and repeat doubling of cells. When consecutive answers of C/C_o vs. time are nearly the same, use coarsest grid yielding the same result. (Note to reader: Realize that this is a modeling exercise only; in reality one would not produce the waste at another well!)

While grids can be rectangular it is advisable to keep the dimensions more or less cubical. In other words no dimension should be more than 2X any other. It is possible to run problems with greater grid variability, however the propensity for truncation errors will most likely increase.

For some reservoir shapes, the number of grid cells in one direction may be twice as many as in the orthogonal direction. Grids should be placed over reservoir shapes so as to maximize the number of "active" cells; i.e. the cells which fall outside the reservoir boundaries are minimized. Cells which fall outside the reservoir boundary are given

zero pore volume in the model, and while they are carried in terms of computer memory storage they are not active in the matrix solution.

Generally, the largest number of rows and columns of cells will occur in the plan view, or areal dimension, of the grid. The number of vertical layers will generally be 10-15 or less while the plan view may contain 20-50 in each dimension. If the number of cells in one dimension of the plan view greatly exceeds the number of cells in the perpendicular direction, there may be computing efficiencies that can be recognized depending upon the numerical solution technique employed. Some techniques, like line successive over-relaxation (LSOR), operate more efficiently when ω, the relaxation parameter, is minimized.

GRID ORIENTATION

The grid should be oriented such that the principles below are satisfied as much as possible. Some of these considerations may lead to conflicting orientations that will require some compromises. These should be based upon the best engineering and geological judgements.

1. Since a simulator usually assumes no-flow boundaries, the limits of the grid should be such that they coincide with the natural no-flow boundaries of the reservoir. For example, pinchouts, sealing faults, etc. are natural no-flow boundaries. A general rule to follow is to superimpose upon the reservoir the largest

possible rectangle that encompasses the entire system. Since the orientation of this rectangle must coincide as much as possible with the natural reservoir boundaries, several rotations about its central axis can be tried before deciding on the best juxtaposition.

2. The grid should be oriented such that it encompasses the active well locations. If infill drilling is anticipated in the future, and the effects of such wells are to be included in the reservoir study, be sure the orientation is such to accommodate the new wells.

3. The orientation of the grid must also account for the principal directions of fluid movement and the natural potential gradients in the reservoir. One should be aware of the grid orientation problem; that is, how the grid is oriented sometimes affects computed breakthrough times, etc. For example, consider the two orientations of the grid in Figure 30.

This figure shows a diagonal and a parallel grid. In the diagonal grid flow always occurs at 45° to the line connecting the wells. In a parallel grid the flow direction is parallel to this line. Frequently, one finds that diagonal grids predict late breakthrough times while parallel grids lead to early breakthrough times. In reality, the actual breakthrough time is somewhere in between these two extremes. For unfavorable mobility

ratios, the difference is particularly severe. The point here is that grid orientation should be recognized and the orientation of the grid should be such that its effect is minimized.

4. The grid orientation should be such that directional reservoir properties are accounted for. That is, the coordinate system should be parallel to the principal axes of permeability as indicated in Figure 30.

Input Data

The form of input data other than grid data will either be tabular or scalar. Examples of tabular data are formation volume factor vs. pressure, solution gas ratio vs. pressure, and viscosity vs. pressure. Normally there are ten or so entries with pressure increments evenly spaced over the entire range anticipated in the simulation.

An example of scalar data is the initial compressibility of water.

Considerable insight to preparation of data is contained in the earlier chapters concerning data requirements and data development.

Output Results

Output of results can occur at each time step, but normally every three, six, or twelve months would be more likely.

Output occurs in two principle forms; 1) well schedule output, and 2) arrays or maps of pressure, concentration, temperature, etc.

Normally well schedule output contains flowing pressures at bottomhole (and perhaps surface) conditions and daily rates. In addition some cumulative data may be kept such as cumulative injected fluid to date. If a waste heat or heat recycling problem is the problem of interest, then wellhead and/or bottomhole temperatures will be listed as well. If concentration of various wastes are important, these may also be noted. If concentration varies over time, then cumulative volumes or mass of waste may be noted.

Arrays of concentration, pressure, temperature, etc. may be useful at the end of each year or so. The frequency of these output arrays may be less than well schedule outputs.

In some cases, a post-processor may be available to draw maps of these array values or plots of pressure, concentration, etc. vs. time at various locations. The more capability the post-processing software has, the easier the interpretations will be.

TIME STEP SIZE

Time step size is sometimes best controlled by observation of changes in certain variables such as saturation (if multi-phase) or concentration (if single-phase). IMPES algorithms solve for pressure by matrix

reduction and concentrations and/or saturations are calculated between pressure solutions (i.e. explicitly). Coefficients of the matrix for the pressure solutions are saturation or concentration dependent and these algorithms are more apt to become unstable and calculate aberrant answers if too large concentration or saturation changes are allowed. For these varieties a 5% change during any time step is as large as should be tolerated for these simulators. Thirty-day time steps are the maximum that should be taken.

If the concentrations and/or saturations are implicitly calculated (along with pressures in the matrix reduction) then layer time steps can be taken. Up to ninety-day time steps or even larger may be all right with implicit simulators.

In addition to aberrant answers one can check the material balance calculations to see if everything is internally consistent. A near 100% material balance should be noted otherwise problems will eventually occur.

MODEL CALIBRATION

Model calibration is the second part of the validation process following simulator verification. The calibration process can proceed once the geologic and petrophysical data have been integrated with the fluid data into the simulator. Simulator verification is the process of validating the mathematics to see if the code is written properly.

Calibration of the model, commonly referred to as "history matching", is the process of adjusting appropriate parameters of the geology, rock properties, and fluid properties until a satisfactory performance match has been obtained between the model's calculated reservoir behavior and the behavior actually observed in the field. Inherent in the discussion of history matching is the assumption that some record of the reservoir's historical injection and pressure performance exists. If injection or production has not occurred in the formation of interest, and if no measurements of natural fluid flow or pressure gradients have been made, then history matching is not possible. Similarly, if injection or production has occurred, but no measurements of reservoir response were recorded, then model calibration from historical measurements is not possible. Examples of measurements of reservoir or wellhead response include reservoir pressure measurements and analysis of produced or sampled fluids.

If some measurements of historical performance data are available, at least partial calibration of the reservoir description may be

possible. The primary purpose of the history matching process is to identify a set of parameters of reservoir description that allows model response to mimic actual performance. Should a large amount of very high quality data be available for a long period of history (several years), it is theoretically possible to reduce the range of uncertainty of parameters, or combinations of parameters, to nearly zero. In this case, the reservoir description would be considered validated. As implied by the phrase "combination of parameters", a unique determination of the individual parameters is not possible under the best of conditions. The technical reason for this fact is that the solution of this so-called "history match" or inverse problem is mathematically non-unique. In actual practice, however, if a model can be constructed while keeping geological and fluid properties within reasonable limits the true parameters are usually approached closely enough. The geologic/petrophysical/fluid picture of the reservoir is clarified a good deal, and the values of parameters throughout the reservoir are within geological reason. This improved definition reduces the possible range of values for these parameters and thus reduces the range of possible results of the simulator. The sensitivity analyses will then be performed within a reduced variation of parameters and the range of results will be closer to the initial results of simulator.

Most data will be available for the injection well or wells of interest. As discussed earlier in the data collection and development process, the more geological and petrophysical data available, the

better. It is during the calibration phase that the model characteristics are refined to reproduce mathematically the actual reservoir performance due to certain injection and production stimuli. For instance, well tests may be performed to produce pressure transients within the reservoir that may be analyzed for reservoir flow capacity (k·h, md. ft.). Depending upon the number of wells at one injection site, it may be possible to run transient pressure interference tests between well pairs from which estimates of interwell flow capacities can be made. Well logs can be analyzed to identify porous zones and flow barriers such as shales or anhydrites. If cores were taken at the time the well was drilled, the resulting core analyses for permeability and porosity should be correlated with logging results. In combination with both logs and transient pressure tests, spinner surveys may be made in individual wells to determine which zones are accepting the injected fluid. Well tests may also be analyzed to see if the sandface of a well is damaged (possibly partially plugged by particulates) or stimulated (carbonate cements or clays dissolved by injecting dilute acids such as that found in pickle liquor). Integration of the data from well tests, logs, cores, and spinner surveys will provide a starting point for a geological interpretation at each well and probably in the interwell distance. Since similar data will not be available at distances far away from the injection wells, some assumptions will have to be made regarding homogeneity in the lateral direction.

During the history matching process it is important to make changes only to reservoir parameters which are poorly known. In addition, these changes must not be allowed to take any parameter beyond its range of uncertainty, that is, to unreasonable values. In general, the injection volumes, rates, and wellhead injection pressures are assumed to be known with accuracy. This data is specified within the model. The comparison parameters of the history matching process may be reservoir pressures and/or phase saturations or constituent concentrations. These values are calculated by the model and compared to actual measurements in the field. The reservoir description is adjusted as required until the calculated values satisfactorily match the measured values. Normally these adjustments will occur in the number of layers, their thicknesses, porosities, and permeabilities.

In some cases where older historical data are involved, the quality of injection records (rates and pressures) may not be as good as more recent records. Reservoirs have "memories", i.e. they will not respond to current injection stimuli properly if the previous "old" data are not included. If older data are poor, the modeler should at least endeavor to inject the correct volumes over time even if exact rates are not known. In this way the material balance concept is preserved. Actual "tuning" or matching of wellhead or bottomhole pressures should be initiated once the data are considered accurate enough to proceed. If an injection well had fifteen years of poor quality data, and data for the last five years were good, one might consider just average rates over the first fifteen years with more

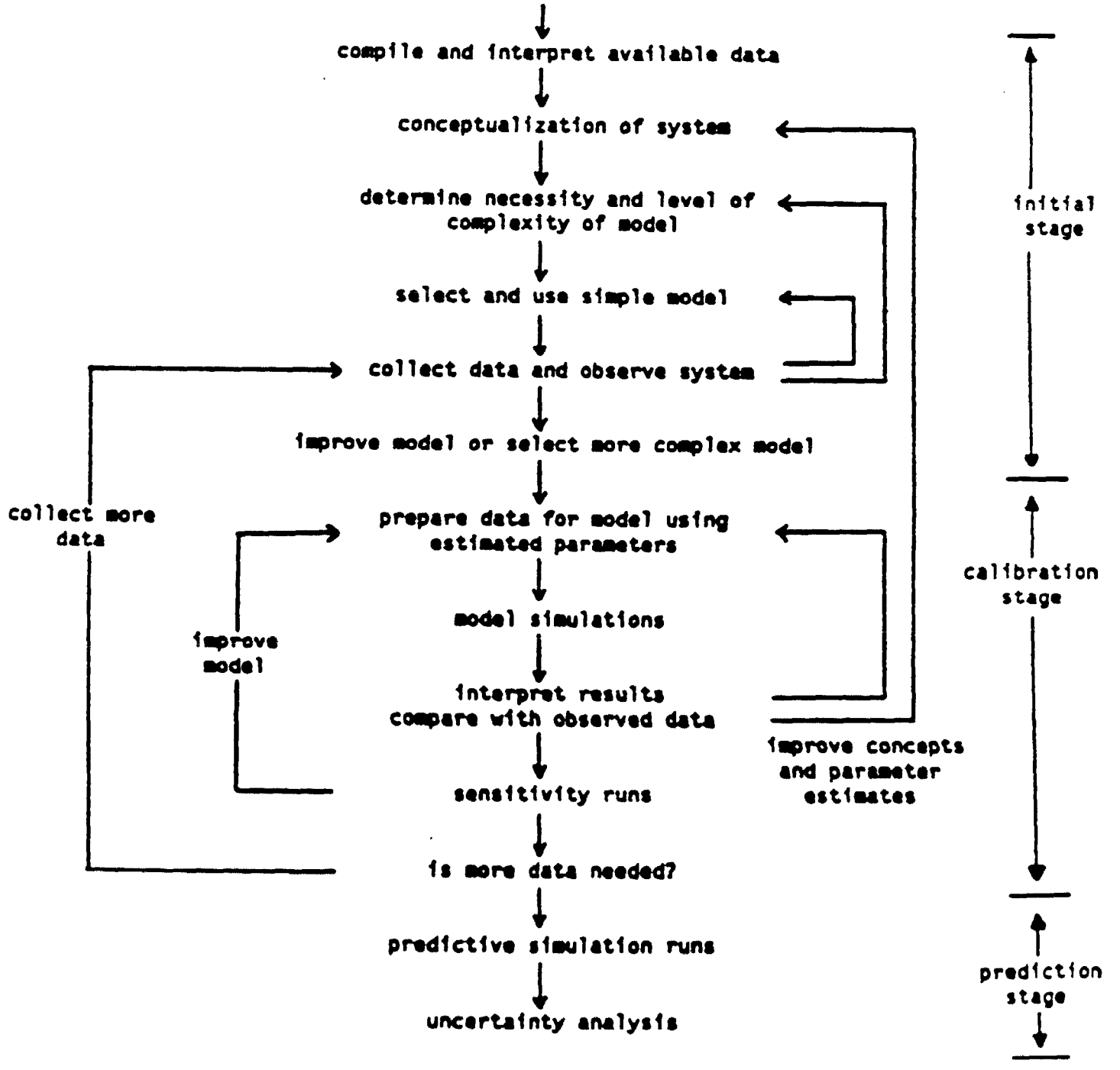
particular attention focused on the last five years as far as pressure matching is concerned. In the case of matching historical pressure one enters the rate data precisely and accepts the model response for pressure at the matching locations as gospel. There is no "universal" guideline for how close (precise) the computer generated pressure response should be to the actual measured pressures. However, if the historical rate records are good with no gaps, and pressures were recorded frequently the discrepancy could be within 10-15%. When rates are changing frequently, or the wells are in service only part of the time, matching will be more difficult.

One problem that is inherent to hazardous waste injection modeling is that geologic and petrophysical data may be available only in the vicinity of the injection well field. Even then, only a few wells clustered in a relatively close neighborhood will be available. Any correlation of layers, etc. between wells will be over a relatively small area. In petroleum reservoir modeling, the wells (production and/or injection) will be distributed over a much larger area; therefore the sources of data will be much wider in distribution. Any data that can be collected from state geological surveys, or the United States Geological Survey, that presents basin wide conceptualization of geology should be utilized to temper the layer thicknesses at distances far away from the injection well site. Insofar as the characterization of individual strata within broad geological layers that are identified from spinner surveys, an assumption will have to be made regarding their homogeneity in lateral extent.

Calibration or history matching is best done as a process revisited after pressure and rate histories are recorded, after additional wells are drilled, after rates have been changed and corresponding pressures noted. Other field tests that can be done are injection and/or fall-off tests, interference tests between wells, etc. A well calibrated model will be able to emulate the actual reservoir pressure responses at various well locations over the complete range of rates and over time once the model is properly constructed. The following table, taken from van der Heijde(1984), illustrates the iterative nature of model calibration as well as incorporation and refinement of data described earlier.

Besides rate impulses and pressure responses, the model should also provide tracking of the concentration fronts of the hazardous waste. One or more constituents may require tracking due to differing reactions with the in situ reservoir water and/or rock fabric. Validation of constituent tracking adds another order of difficulty to the overall history matching process. The rock acts as a chromatographic column in some respects except in addition to adsorption/desorption and holdup, some transformation of one or more injected chemicals may also occur. Coreflooding in a laboratory environment with actual core from the geological horizon of interest is the only way to closely approximate the in situ reservoir conditions. Coreflooding must be done at the same conditions of temperature and pressure as exist in actual reservoir. The same in situ water chemistry must be synthesized and the same hazardous waste must be injected at rates approximating the actual rates used in the injection well.

MODELING PROCESS [from van der Heijde(1984)]



Effluent concentrations of several ions should be monitored until the overall chemistry is understood. The model used in the field can be used to model the 1-D lab experiments with the most emphasis on tuning the chemical kinetics. Once the process variables and reaction kinetics are in hand the same reaction kinetics can be combined with the field geological description to produce the calibrated field model.

Field tests of concentration fronts could vary from injection/production cycles in the same well or bottomhole sampling at an observation well while injecting nearby.

During all of the phases of history matching, a log of the trial runs should be kept in order to avoid duplicating simulations made earlier. Sometimes a change is suggested to the user following a combination of trial runs that a single run will not suggest.

There is always some uncertainty in predicted performance. The objective of calibration or "history matching" is to utilize all data available, to make the data as consistent between data sources (logs, cores, well tests, etc.) as possible, and to be thorough in the construction of the model. If all sources of data have been exhausted, and the analyst has been thorough and workman-like, then the resulting waste flow predictions are probably as good as can be expected. One can perform sensitivity analysis work (discussed in the next chapter), and if lack of historical injection data is a weakness, a recalibration can be performed as soon as another year's worth of

data are accumulated. In fact, a recalibration of the model should be done at any time that the actual performance seems to deviate widely from that projected by the model.

SENSITIVITY ANALYSIS

GENERAL

If insufficient historical performance data is available to calibrate or improve the reservoir description of the model, the history matching process is eliminated and the full weight of calibration falls on sensitivity analyses. These analyses consist of a series of runs in which the parameters controlling flow of the injected fluids are varied within their range of accuracy. If the simulator indicates that the hazardous wastes are contained within the injection zone, despite changing these parameters to extremes of their range of possible values, actual containment of these wastes in the field can be assumed with some confidence. It should be emphasized here, however, that even a well performed sensitivity analysis is not nearly as revealing as a good history match (providing the data are available for a history match). Sensitivity analyses are discussed in detail in the following section of this manual.

WORST CASE APPROACH

Without the benefit of historical data, and in light of the need to investigate the spread of hazardous waste in a subterranean reservoir, what measures can we take to alleviate the long term concern for containment? Perhaps the best approach to this problem is a "worst case" approach. Let us examine those parameters which could

exacerbate the spread of waste and utilize all of those parameters in one prediction run. The probability of the worst case is most likely low; however if we do not have data perhaps this is the best starting point. One thing seems fairly certain; if containment is accomplished in this simulation then it most likely will be true for the real case.

The reservoir description parameters most likely to cause far reaching spread of injected waste are 1) heterogeneous permeability layers in the storage zone, 2) leaky aquitards above and below the storage zone combined with high injection pressures, 3) low porosity in the storage zone, 4) lack of chemical reactions, 5) high density differences between injected and in situ fluids, and 6) high dispersion between injected and in situ fluids in the storage zone.

Heterogeneous bedding plane permeabilities may be characterized by Dykstra Parson coefficients of 0.9 or more. With high contrast in permeability one or two thin high permeability zones will transport large amounts of injected waste large distances, while the spread of waste will be retarded in the low permeability zones.

Aquitards which form the underburden and overburden layers are normally comprised of shales and/or anhydrites. These barriers are characterized by low permeability values between 0.000001 and 0.01 md and will leak at high injection pressures over long times. Miller et al (1986) utilized the Hantush and Jacob leaky aquifer theory for order-of-magnitude estimates of final permeation distance. This theory

ought to provide quick estimates of the leakage distance over long periods of time. The addition of high injection pressures may worsen the Hantush permeation distance estimate; this factor needs further investigation.

Low storage zone porosities are more rapidly filled with waste thus causing outward movement earlier in time.

Inability to characterize degradation or transformation reactions disallows their use in aquifer storage modeling. Therefore hazardous material will be assumed to travel forever unabated by reaction with underground fluids or rock fabric.

High density differences will cause under- or over-running of waste depending upon other rock properties being utilized. High vertical to horizontal permeability ratios allow natural convection to come into play especially at large distances from injection wells where fluid velocities are low.

High values of dispersion can also amplify the spread of waste, particularly in highly heterogeneous layers with low vertical/horizontal permeability ratios. With higher vertical/horizontal permeability ratios and high transverse dispersion between fluids of nearly equal density the frontal displacement profile of injected waste may actually be flattened.

Various combinations of the aforementioned variables should be experimented with to see which variables cause the biggest distortion in the spread of waste. The best approach to this testing is to establish a "base case", perhaps the one felt most probable, and then vary only one parameter at a time in each simulation. Otherwise, if more than one parameter is varied, you will never be able to identify the specific cause of the changes which result. In this way one will be able to isolate the variables which need the greatest work in the determination of specific value. Other variables may be estimated much more loosely since the effects of their changes are less onerous. Some quick simulations over large ranges of the variables at the outset of the study will quickly focus the investigation on the most important variables. Once the more sensitive variables are identified, a "maximum worst case" can be run by adjusting all parameters to their worst case values from the single variable runs and making a final simulation.

PREDICTION OF FUTURE PERFORMANCE

Once model calibration is complete future performance prediction is reasonably straight forward.

Injection rates will be specified together with time step length and number of time steps. If formation parting pressure is thought to be a consideration at some future time, a maximum flowing bottomhole pressure should be specified for injection wells. It is unlikely that over pressuring of the reservoir to the point of rupture will occur, but one should be aware of the condition in the simulations. There is nothing mathematical that will happen if this over-pressured condition is reached so some mental reminder should be in place. If the flowing bottomhole pressure constraint is invoked, the rate will be reduced by the simulator if the wellbore pressure condition is approached. So long as the wellbore pressure condition for injection is limited by the user to a pressure less than the formation parting pressure, no violation of this physical condition will occur.

Time step sizes should be kept at about thirty (30) days for most models during prediction; however, sixty (60) to ninety (90) days may be possible. The user should examine material balance numbers at each time step to see if any appreciable error is occurring or beginning to get large. Most codes have a time step adjustment based upon the change in concentration or on material balance. As long as no abrupt changes in operating conditions are made, longer time steps will be

automatically made by the simulator. A time step size should be utilized to keep material balances at 99-100%. Since the economic life of most injection projects will be no more than 30-35 years, simulations of this operating life should still be economic to perform.

For simulations as long as 30-35 years several restart records will be desirable. A restart record contains all of the simulator data to perform another time step and is dumped to a disk or magnetic tape file for restarting at a later time. The simulation of predicted performance will be done in time periods, and it will be possible to review these before executing the next time period. These reviews will be useful since any problem observed early-on that is undesireable can be corrected and a rerun made before proceeding.

It is important that the correct wellbore mechanics are in the model and in concert with the actual field performance before starting the prediction. Sometimes, depending upon the constraints utilized in history matching, the initial wellbore conditions for prediction may be changed. For instance, during history all injection rates are known so history match runs frequently are made by varying reservoir properties until a flowing bottomhole pressure match is observed. During a prediction, it may be easier to specify a flowing bottomhole pressure and let the model calculate all future rates. If pressure and rate boundary conditions are exchanged at the time a prediction is begun, then one should use some care in checking to be sure the prediction begins with properly calibrated wellbore mechanics.

For 10,000 year estimates the expense of numerical simulation will be prohibitive. Once the concentration maps for waste spread are developed over an operating lifetime the only convective force remaining in the storage aquifer will be the velocity or "drift" caused by recharge at the surface or from underground flow between two points or areas of differing potential heads. Since this velocity will be relatively constant for long periods of time, a hand calculation using a steady-state version of Darcy's law should suffice for the 10,000 year containment estimate in many cases.

The maximum vertical distance that waste should traverse will be located in the reservoir layers (both in confining and other aquifer layers) just above an injection wellbore. The time of maximum advance of "leak" in this vertical direction will occur shortly after the end of the operating lifetime of a waste storage project. At the moment the last injection well is shut-in, a steady-state (or nearly steady-state) cone-shaped potential field (pressure or head) will exist above each injection well. This pressure cone will dissipate rather rapidly after the injection wells are shut-in at the end of the project and the advance of further leakage will diminish. The simulator of interest should be capable of presenting iso-concentration contours resulting from this vertical leakage. The maximum advance of waste leakage will be visible in these iso-concentration maps. Since leakage into or through confining aquitards will be very slow (at low velocities), convection will control the leakage process. There is no need to

consider dispersion in the leakage calculations since dispersion is directly dependent on the leakage velocity which will be quite low.

The final results of a prediction are of course the concentration map (or array) of injected waste. Since over- and under-burden layers will be included in the model, one can check the permeation distances and concentrations at those distances to see if the containment criteria have been met or whether further work must be done. If a "worst case" criterion is met, containment may be considered accomplished and the simulation work completed. Otherwise it may be necessary to improve the precision of the more important variables and try again.

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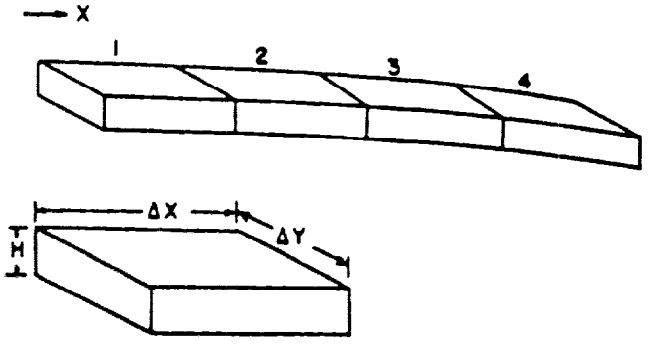
LIST OF FIGURES

Horizontal



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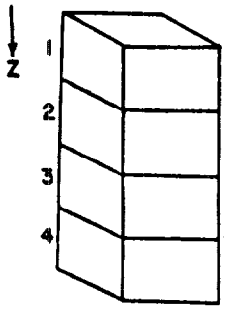
KMAX = 1

CELL DIMENSIONS

Example Applications

- simple "material balance"
- simulates sections of reservoirs
- aquifer behavior
- used in specialized studies, e.g. line drive
- simulate lab experiments

Vertical



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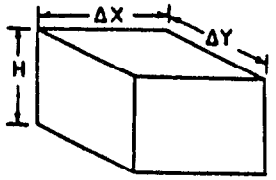


CELL DIMENSIONS

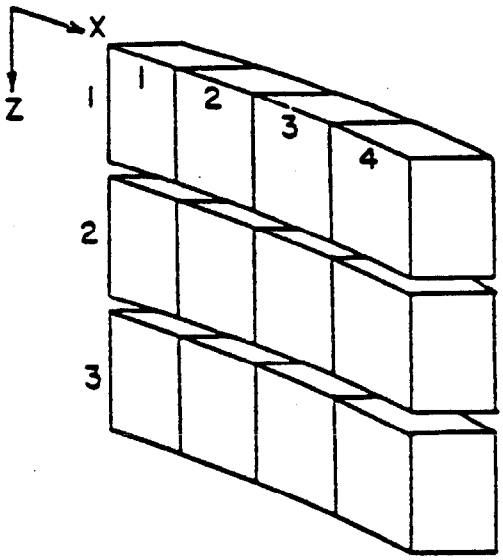
Example applications

- simulates gravity drainage systems
- reef structures
- vertical equilibration
- single well operation
- vertical water influx efficiency

1-D MODEL

SCIENTIFIC SOFTWARE-INTERCOMP

Figure 1



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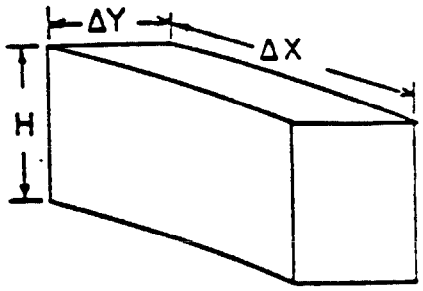


CELL DIMENSIONS

Example Applications

- vertical cross-section studies
- multiple completion wells
- commingled production practices
- stratified flow patterns

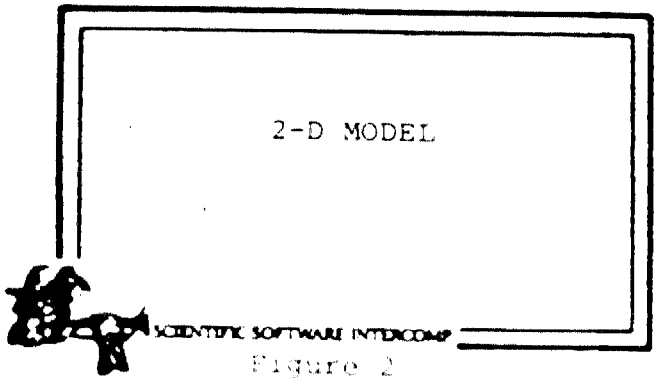
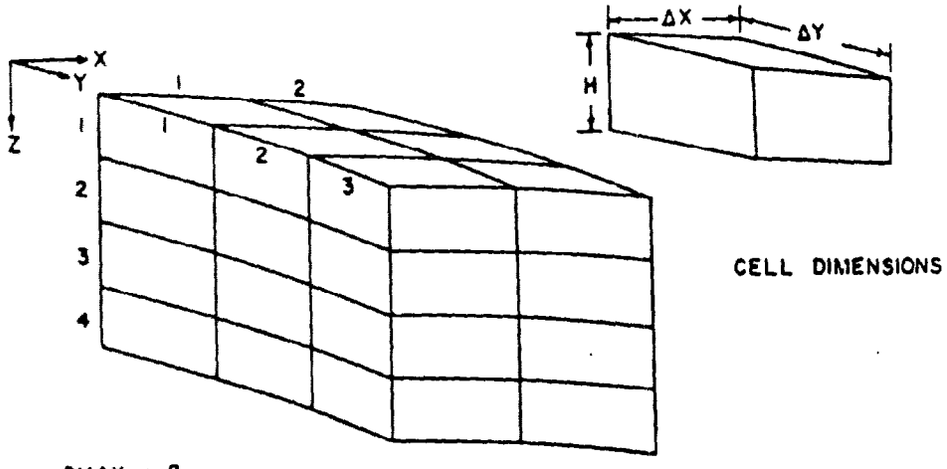


Figure 2

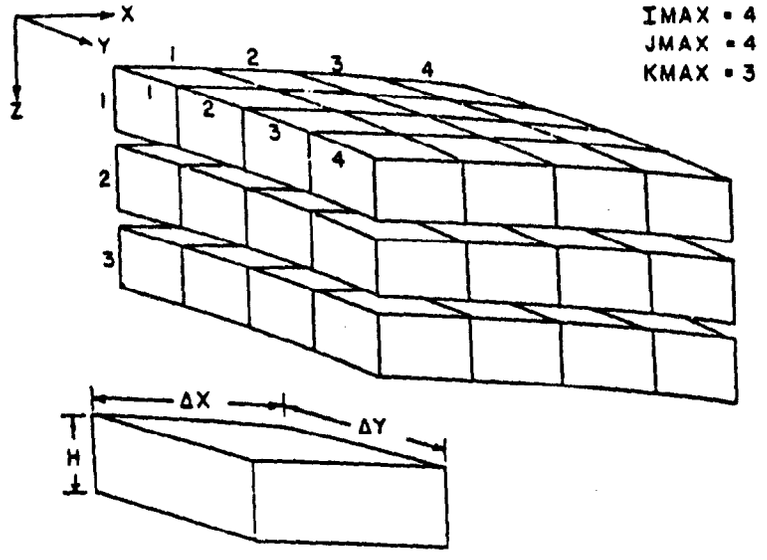
Communicating Layers



Example Applications

- simulation of large multi-well reservoirs
- thick reservoir pay sections
- significant vertical variation in rock and fluid properties
- layered system with common aquifer or partial communication

Noncommunicating Layers



Example Applications

- simulation of large reservoirs consisting of several producing horizons
- no vertical cross flow between layers
- multiple completions with or without commingled production
- stratified flow patterns

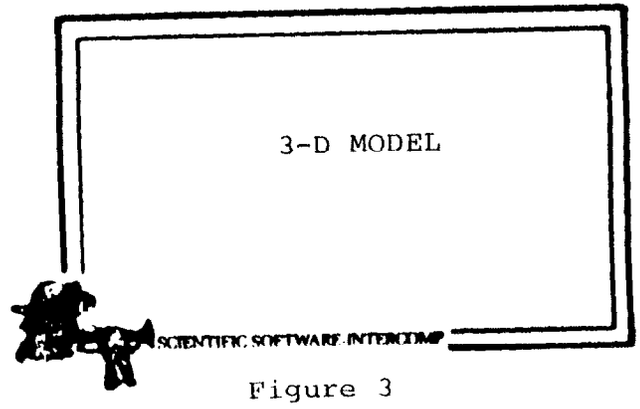
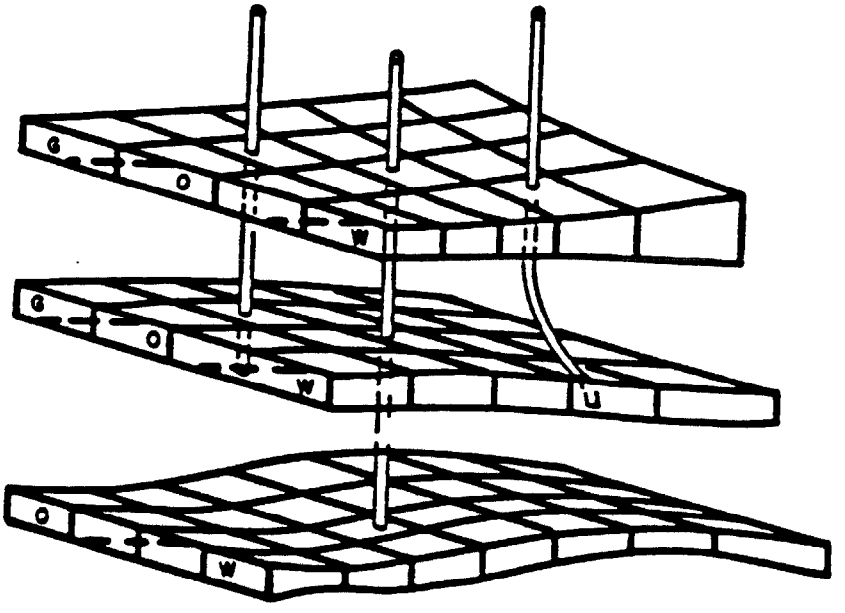


Figure 3

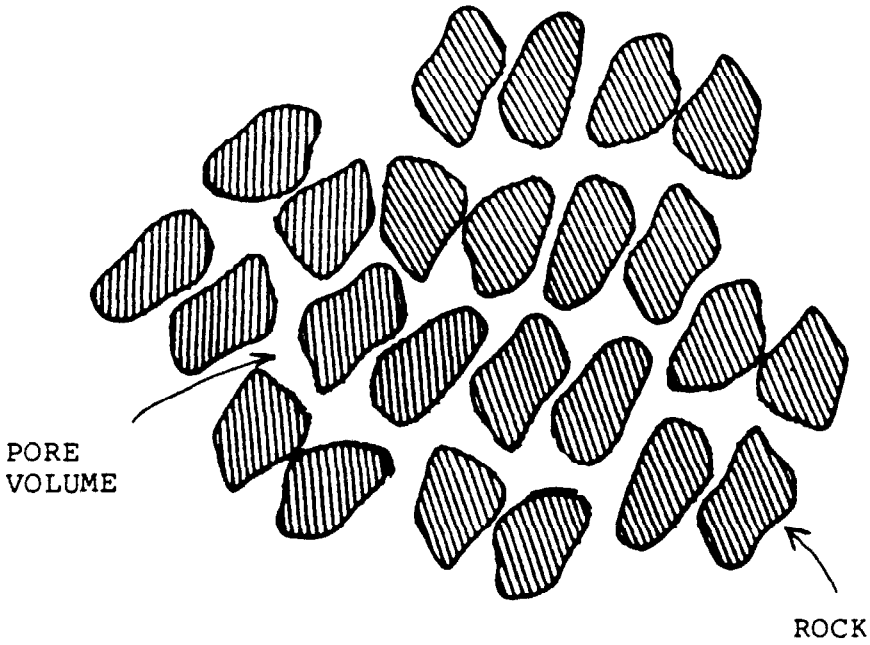


3-D MULTIPLE WELL

COMPLETION MODEL

SCIENTIFIC SOFTWARE INTERCOMP

Figure 4

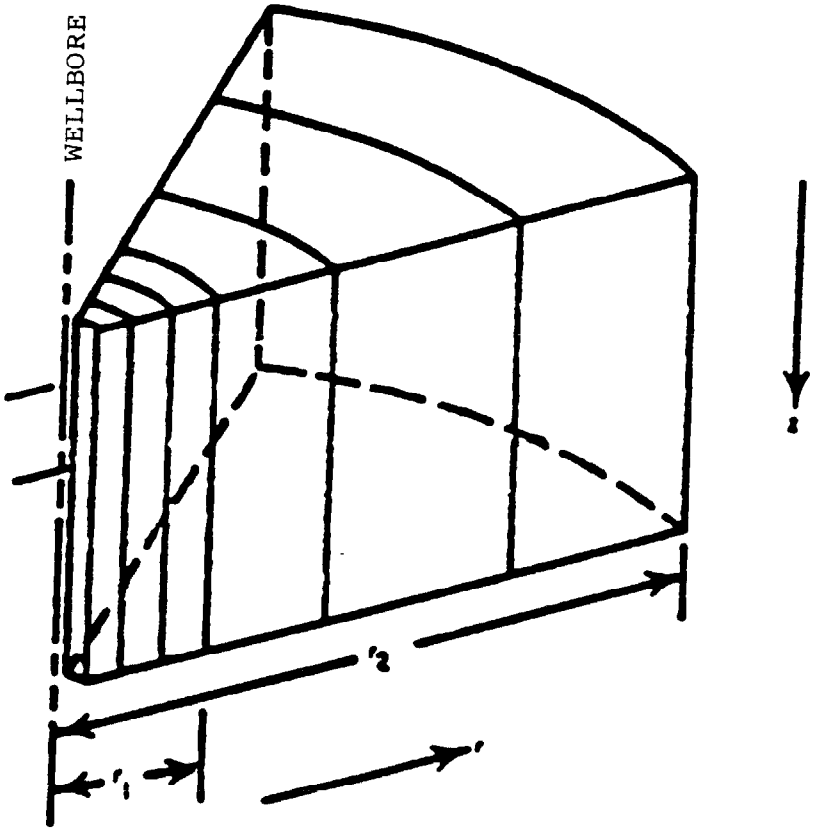


SCHEMATIC OF PORE

VOLUME

SCIENTIFIC SOFTWARE INTERCOMP

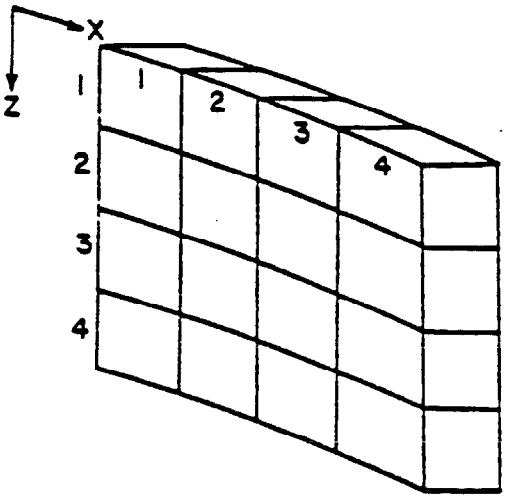
Figure 5

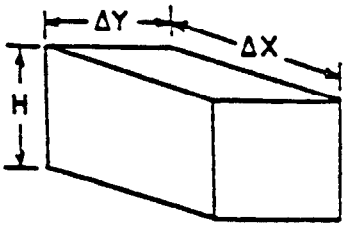


1-D RADIAL MODEL

SCIENTIFIC SOFTWARE INTERCOMP

Figure 6





CELL DIMENSIONS

IMAX = 4

JMAX = 1

KMAX = 4

Example Applications

- cross-section analysis of a reservoir
- gravity segregation effect
- single or multi-well analysis
- heterogeneity effect on frontal displacement

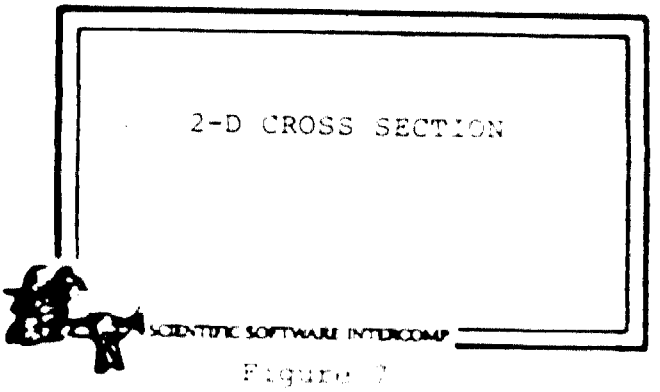
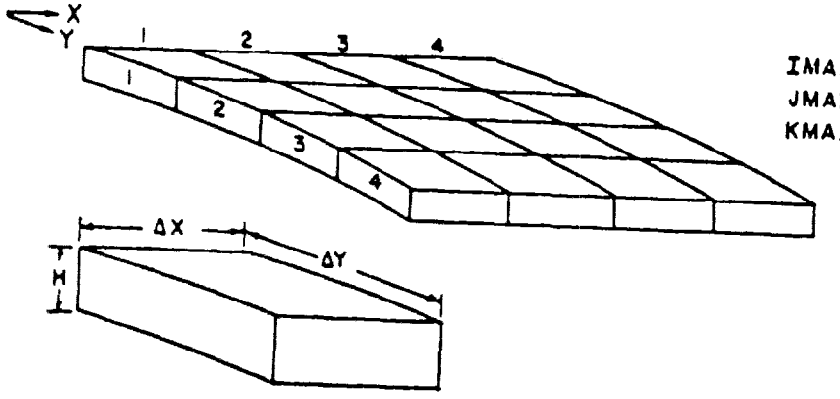


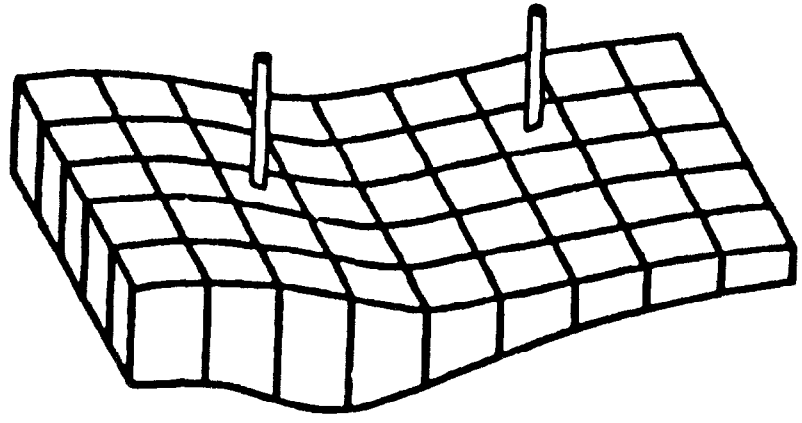
Figure 7



CELL DIMENSIONS

Example Applications

- simulation of large multi-well structures
- heterogeneous rock properties
- small vertical variation of rock and fluid properties
- migration of fluid analyte across lease lines
- selection of optimum pressure maintenance and secondary recovery mechanism



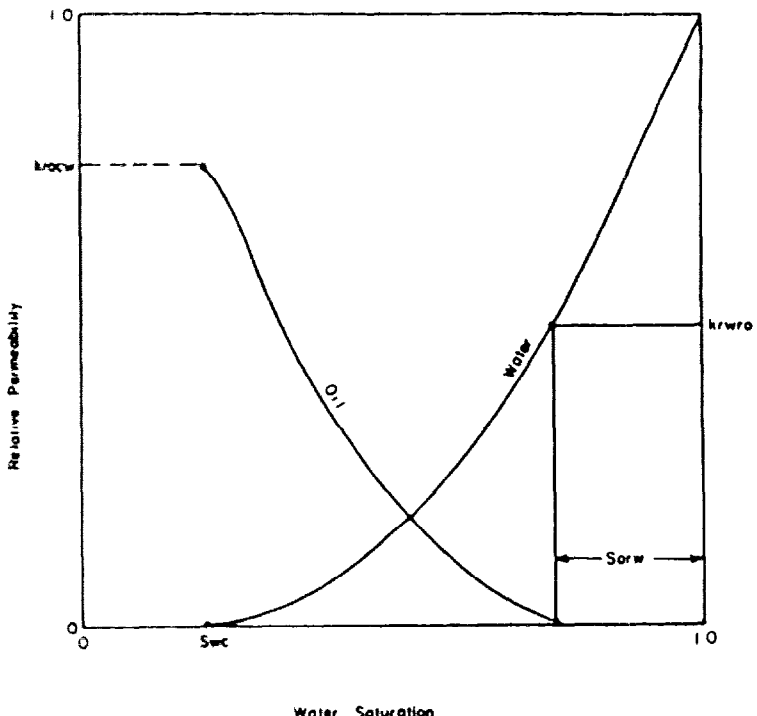
Variable Bed Thickness

2-D AREAL MODEL

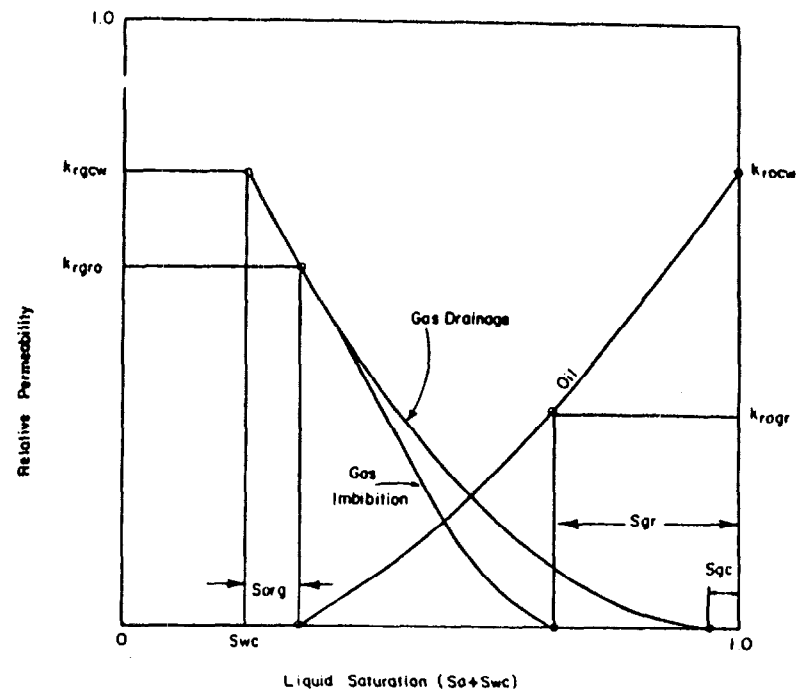
SCIENTIFIC SOFTWARE-INTERCOMP

Figure 8

WATER-OIL RELATIVE PERMEABILITY CURVES



GAS-OIL RELATIVE PERMEABILITY CURVES



where:

S_{wc} = connate water saturation

S_{orw} = residual oil saturation to waterflood

k_{rocw} = relative permeability at S_{wc}

K_{rwro} = relative permeability at S_{orw}

S_{gr} = residual gas saturation

S_{gc} = critical gas saturation

S_{org} = residual oil saturation to gas

K_{rgcw} = relative permeability to gas at connate water

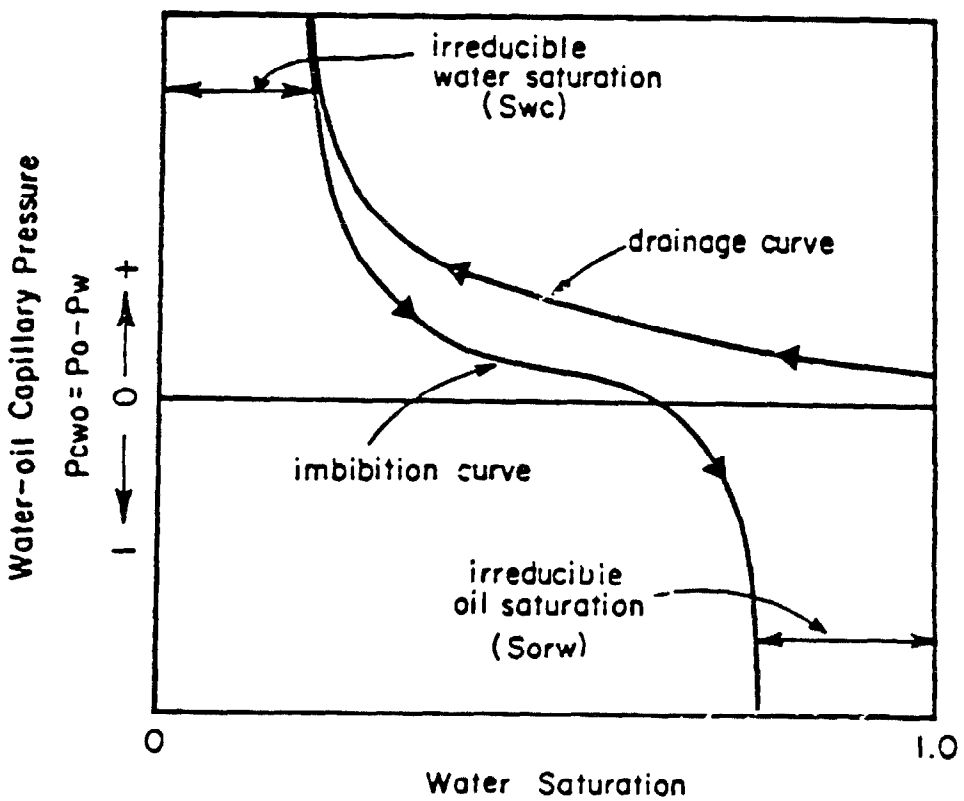
K_{rgro} = relative permeability to gas at $1-S_{wc}$

TYPICAL RELATIVE PERMEABILITY CURVES

SCIENTIFIC SOFTWARE INTERCOMP

Figure 9

TYPICAL WATER-OIL CAPILLARY PRESSURE CURVES



where:

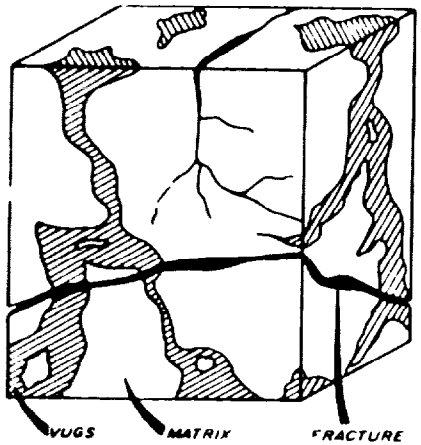
Po = pressure in oil phase

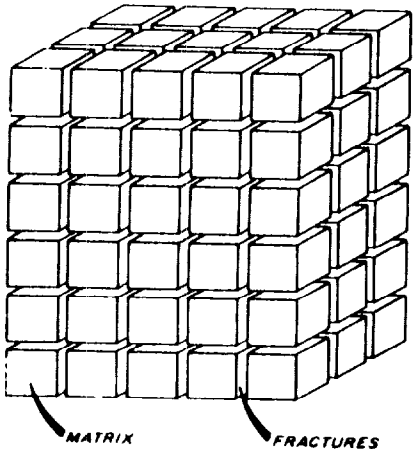
Pw = pressure in water phase

WATER-OIL CAPILLARY CURVES

SCIENTIFIC SOFTWARE INTERCOMP

Figure 10

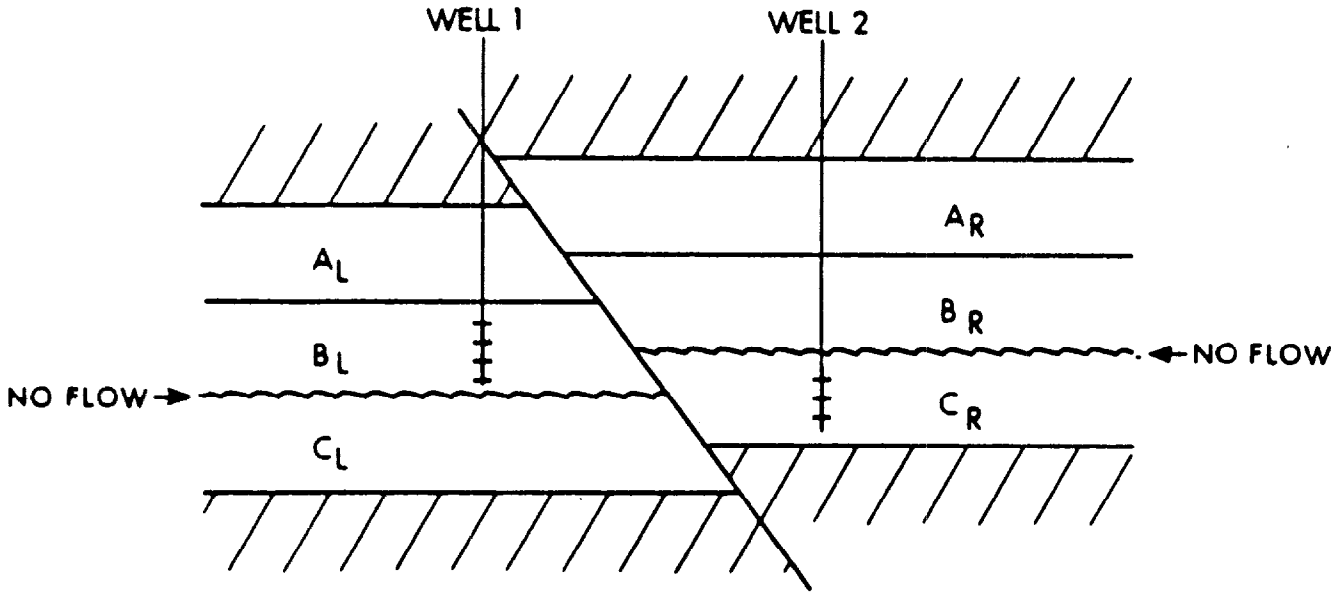




DUAL POROSITY RESERVOIR
AND MODEL SCHEMATIC

SCIENTIFIC SOFTWARE INTERCOMP

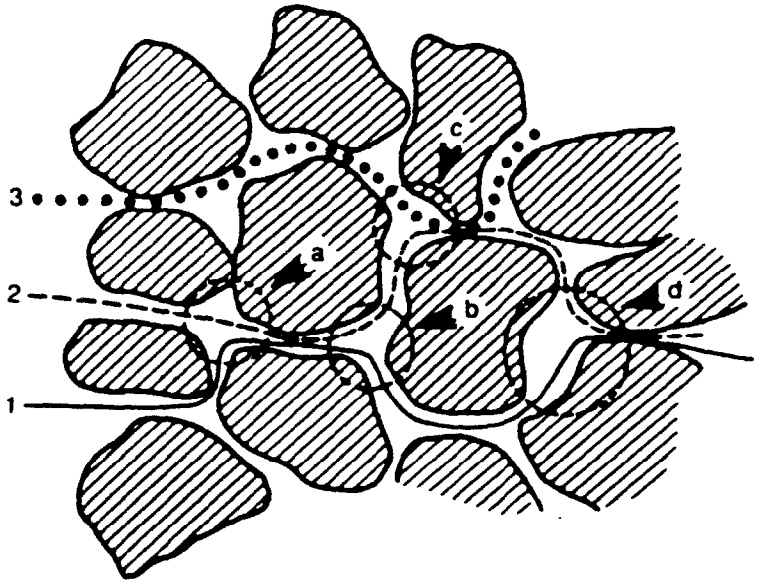
Figure 11



EXAMPLE OF A FAULT

SCIENTIFIC SOFTWARE INTERCOMP

Figure 12



A, B, C, and D = Pore Space Mixing Cells

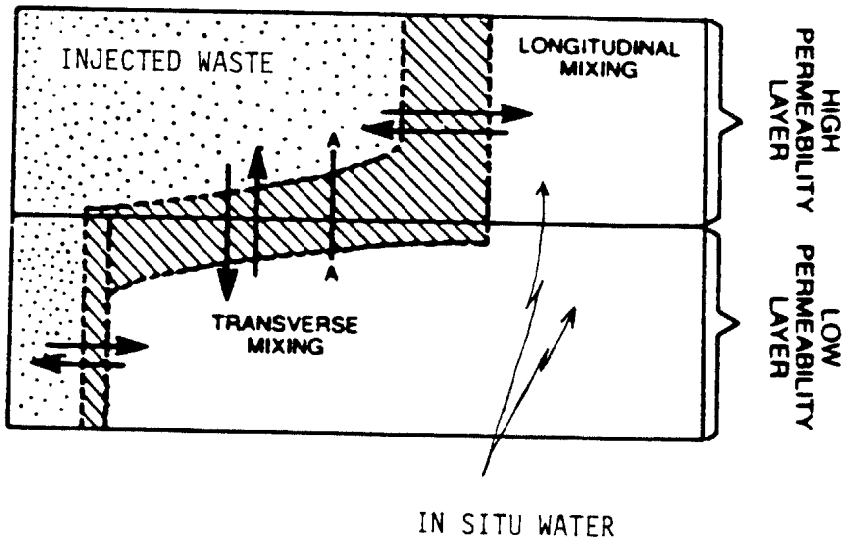
1, 2, and 3 = Stream Lines

MICROSCOPIC CONVECTIVE DISPERSION

after Stalkup, F.I., 1983

SCIENTIFIC SOFTWARE INTERCOMP

Figure 13

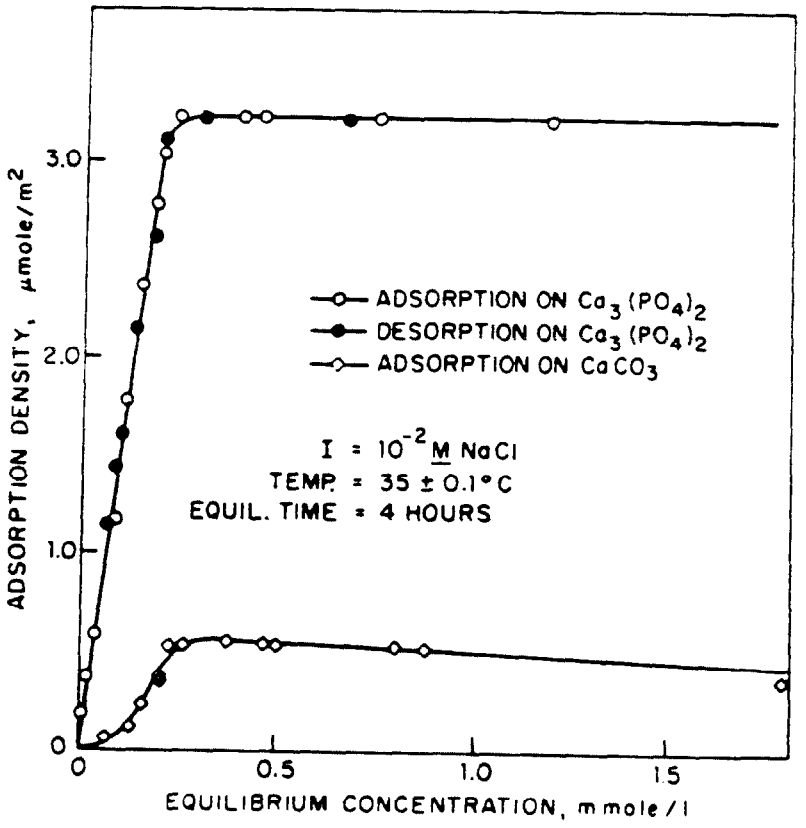


EXAMPLE OF TRANSVERSE AND LONGITUDINAL DISPERSION

After Stalkup, F. I., 1983

SCIENTIFIC SOFTWARE INTERCOMP

Figure 14



Adsorption isotherm of cetyltrimethylammonium bromide (CTAB) on tricalciumphosphate and calcium carbonate

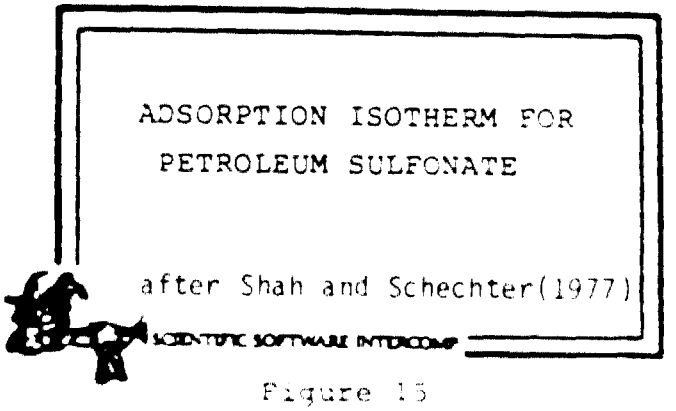
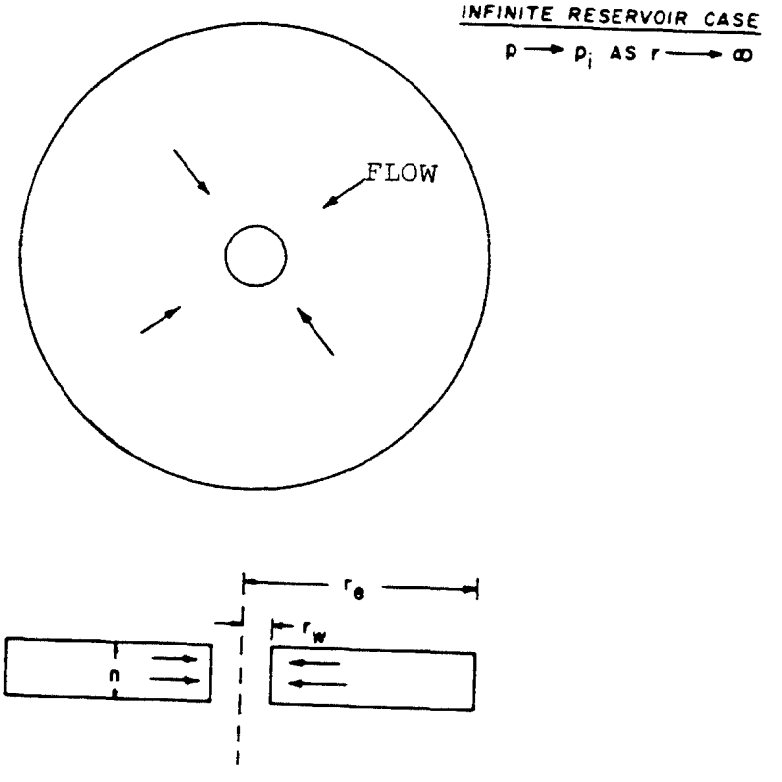


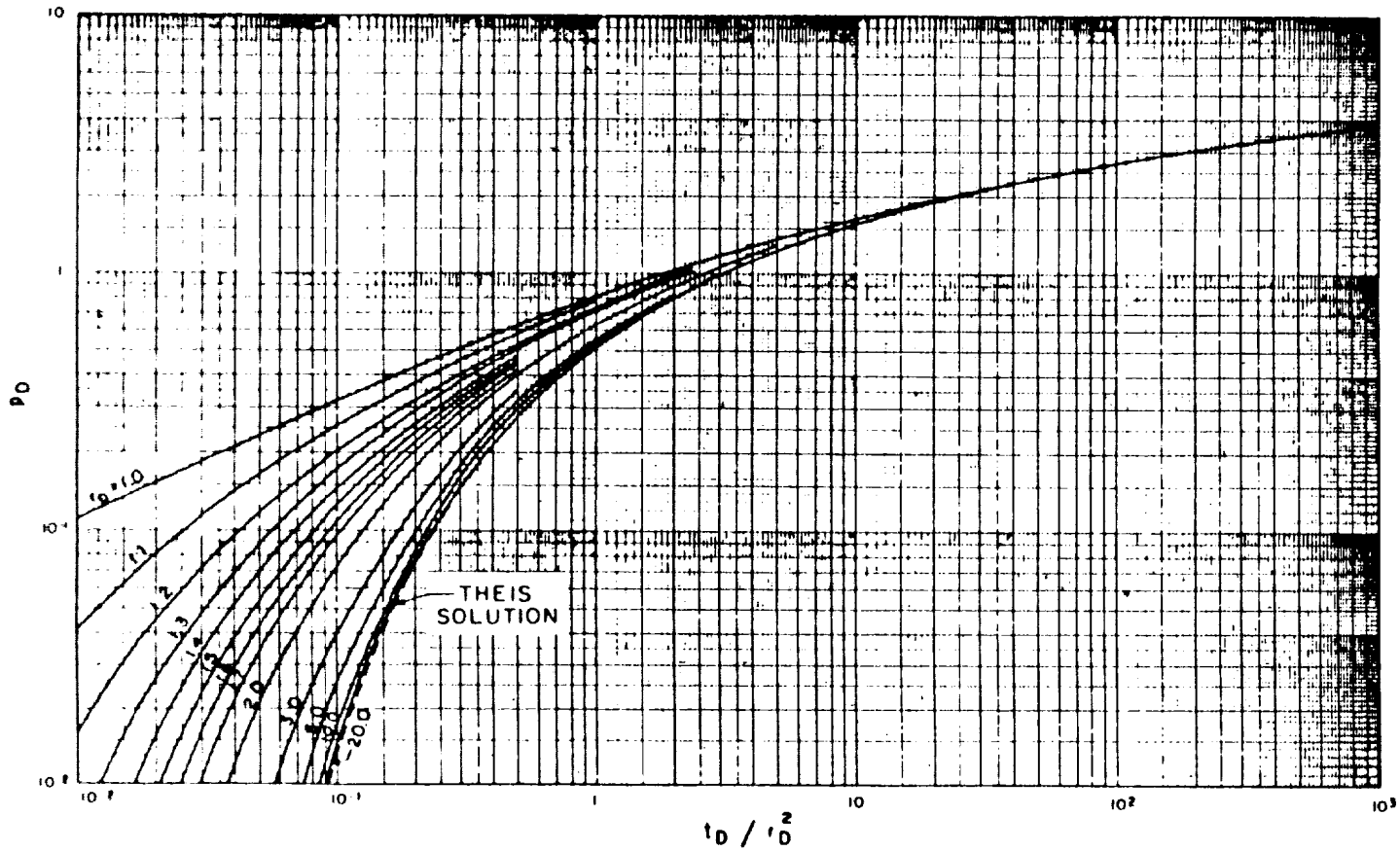
Figure 15



SCHEMATIC OF SINGLE WELL IN AN INFINITE SINGLE PHASE SLIGHTLY COMPRESSIBLE FLUID

SCIENTIFIC SOFTWARE INTERCOMP

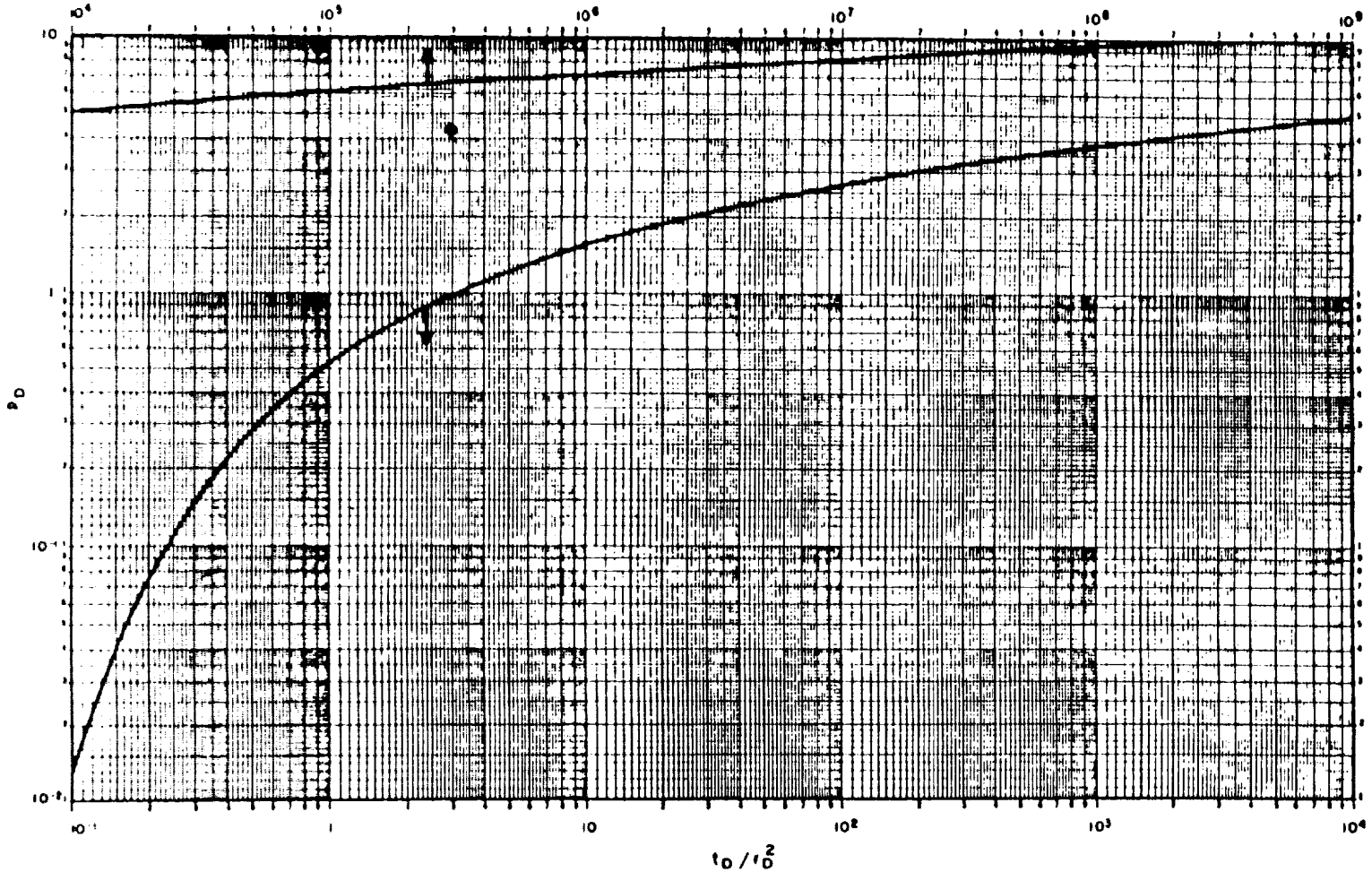
Figure 16



DIMENSIONLESS PRESSURE
FOR A SINGLE WELL IN AN
INFINITE SYSTEM,
SMALL r_D
after Mueller & Witherspoon

SCIENTIFIC SOFTWARE-INTERCOMP

Figure 17

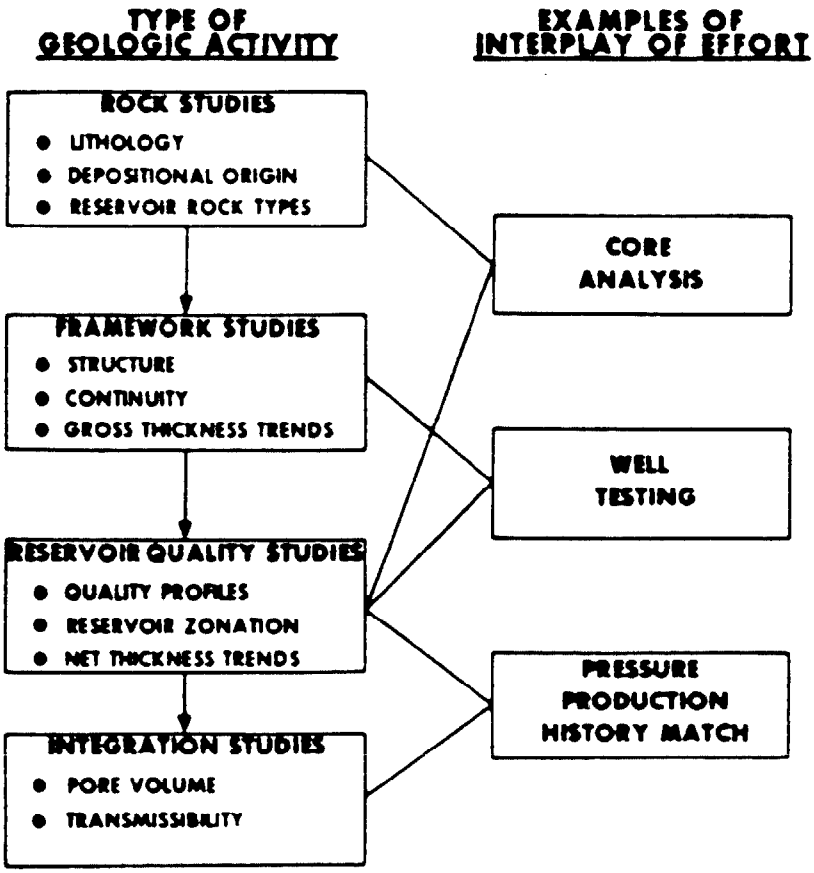


DIMENSIONLESS PRESSURE
FOR A SINGLE WELL IN AN
INFINITE SYSTEM

"THEIS SOLUTION"
after Mueller & Witherspoon

SCIENTIFIC SOFTWARE-INTERCOMP

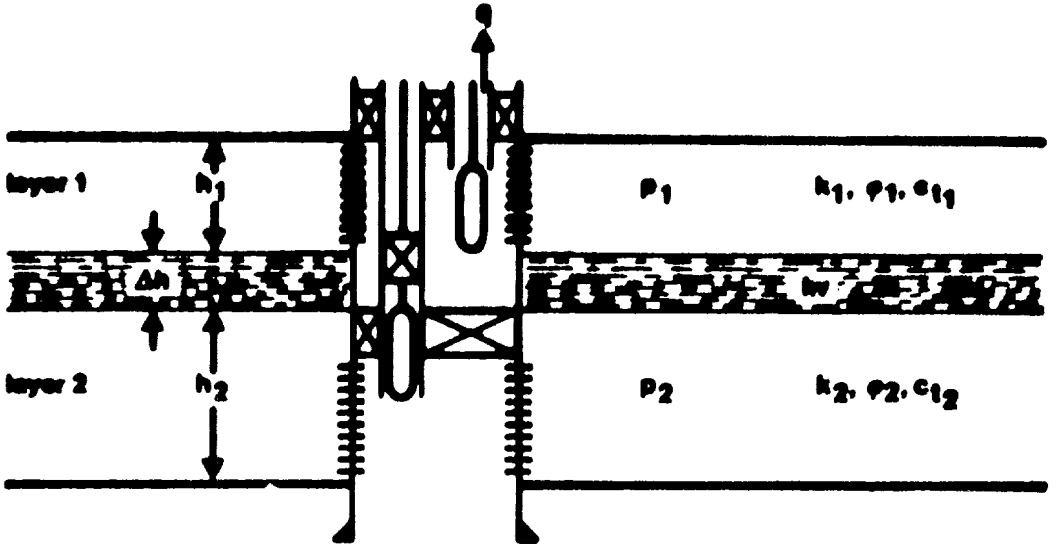
Figure 18



GEOLOGIC DESCRIPTION
FOR
NUMERICAL SIMULATION

after Harris, D.G., 1975
SCIENTIFIC SOFTWARE INTERCOMP

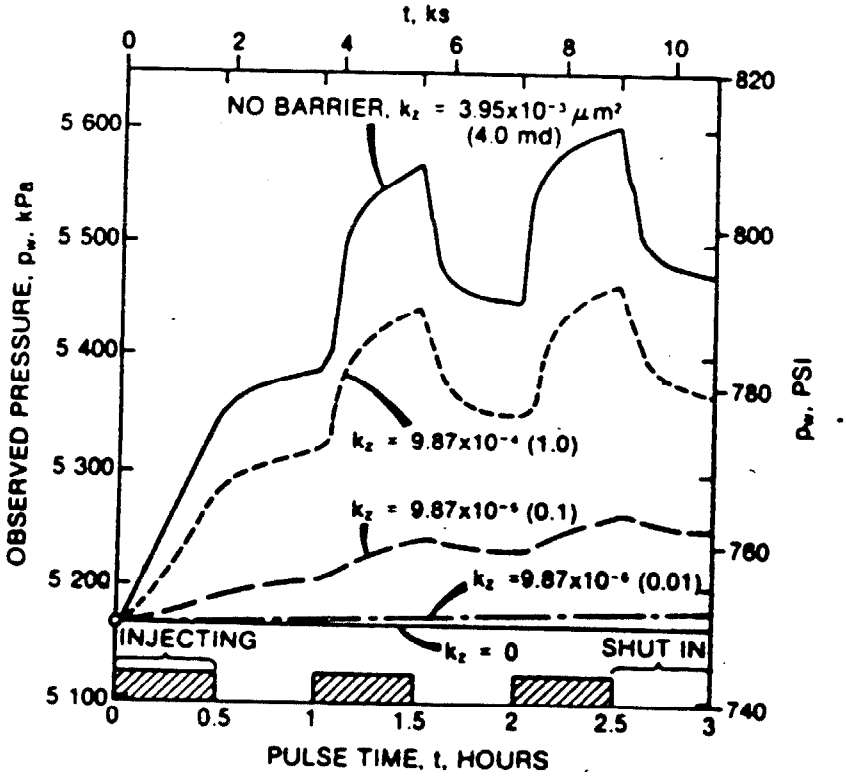
Figure 13



MODEL FOR SINGLE WELL
VERTICAL INTERFERENCE TEST
ACROSS A TIGHT ZONE

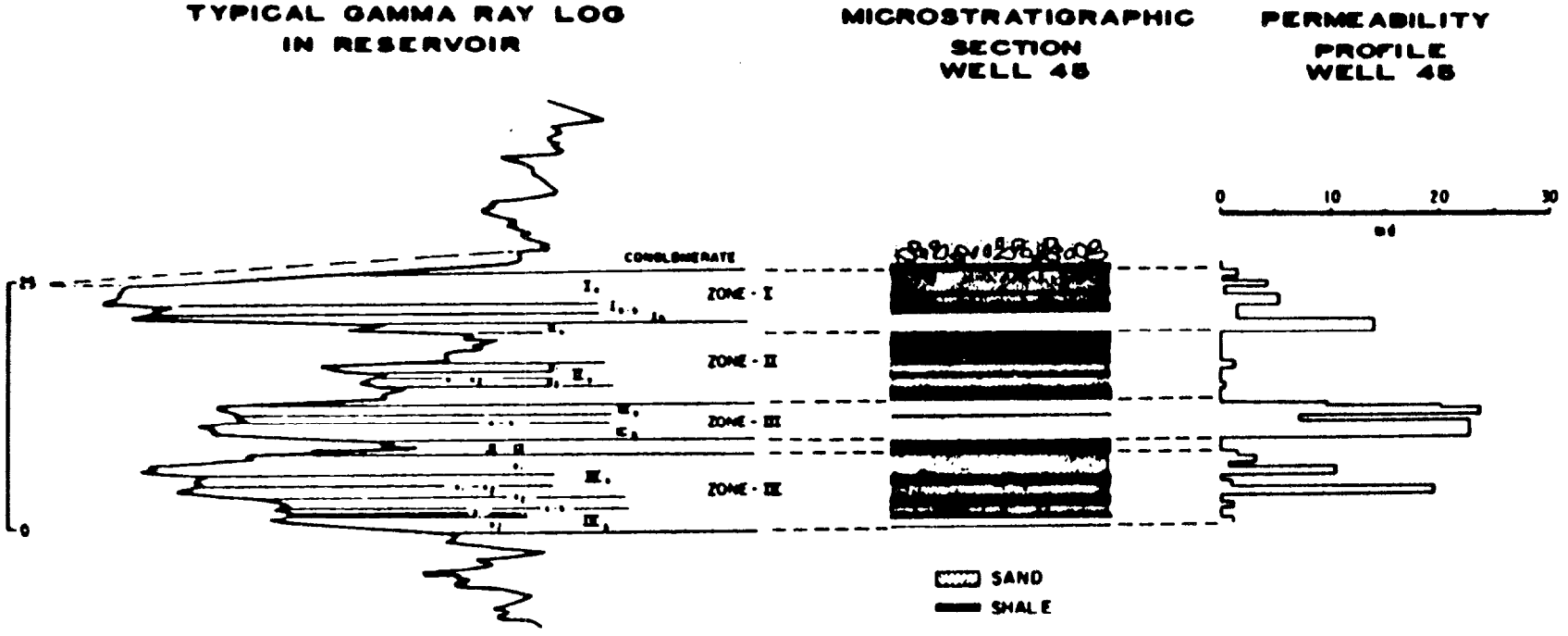
SCIENTIFIC SOFTWARE INTERCOMP

Figure 20



SIMULATED PULSE TEST BEHAVIOR FOR SEVERAL BARRIER PERMEABILITIES

(adapted from Earlougher)

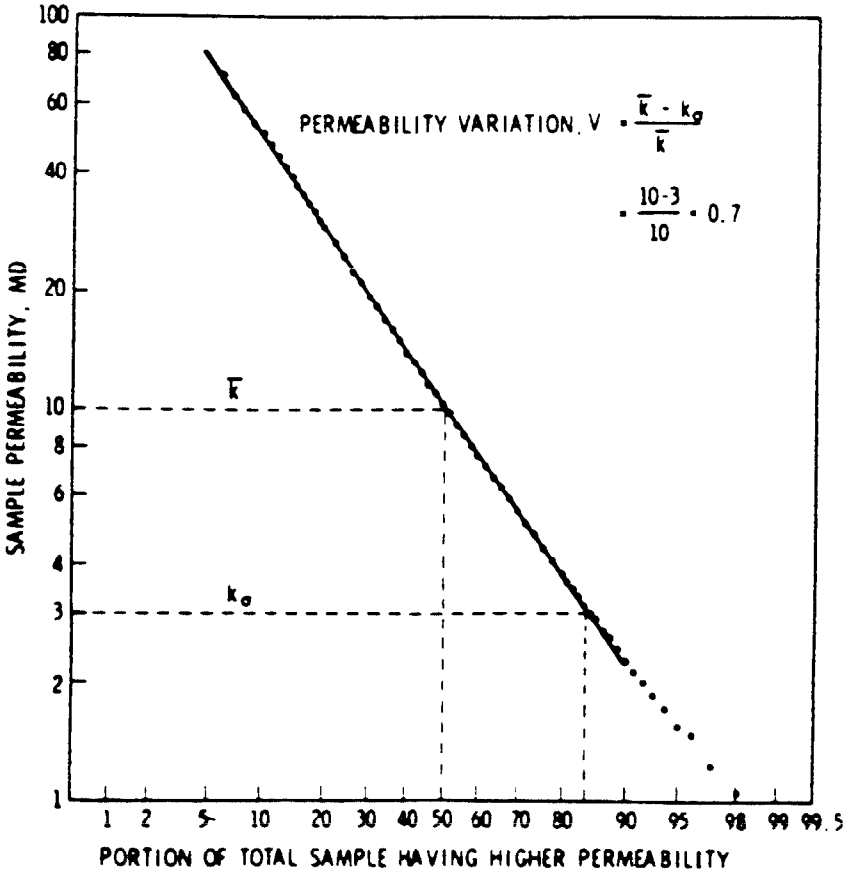


EXAMPLE OF PERMEABILITY VARIATIONS

after Alpay, O.A., 1972

SCIENTIFIC SOFTWARE INTERCOMP

Figure 22

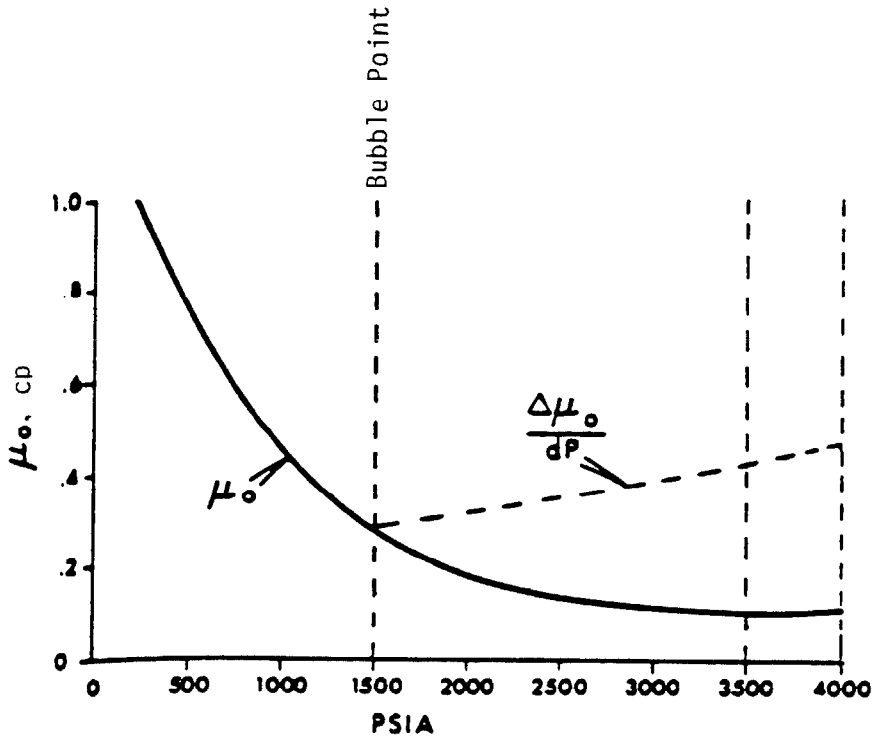


V_{DP} VS SAMPLE PERMEABILITIES

After Craig, F.F., 1971

SCIENTIFIC SOFTWARE INTERCOMP

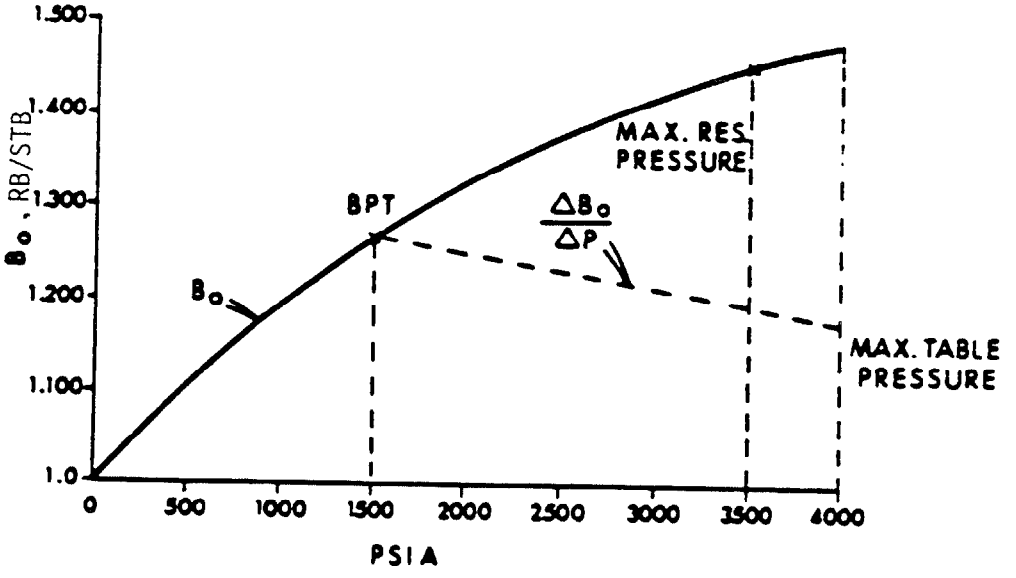
Figure 23



VISCOSITY VS PRESSURE

SCIENTIFIC SOFTWARE INTERCOMP

Figure 14



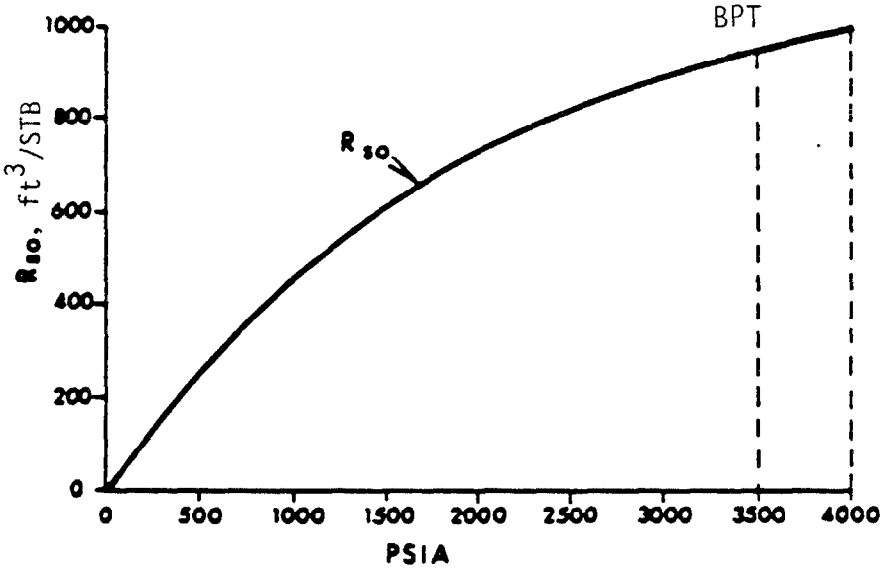
FORMATION VOLUME FACTOR (B_o)

VS

PRESSURE

SCIENTIFIC SOFTWARE INTERCOMP

Figure 35



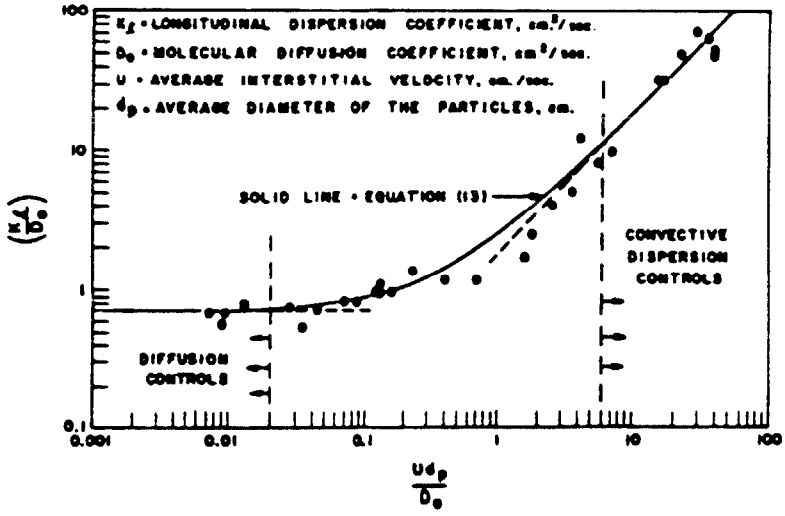
SOLUTION GAS OIL RATIO (R_{SO})

VS

PRESSURE

SCIENTIFIC SOFTWARE INTERCOMP

Figure 26

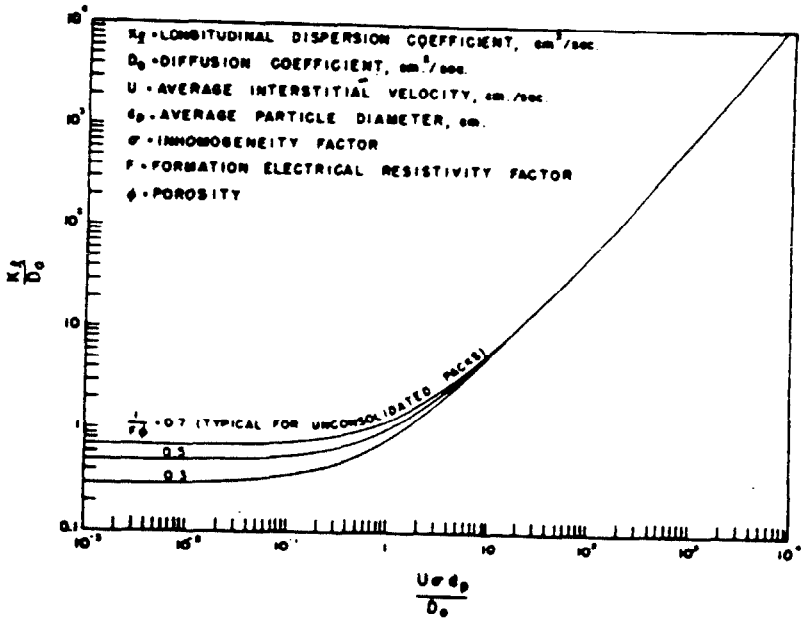


LONGITUDINAL DISPERSION COEFFICIENTS FOR UNCONSOLIDATED, RANDOM PACKS OF UNIFORM SIZE SAND OR BEADS

(after Perkins & Johnston)

SCIENTIFIC SOFTWARE INTERCOMP

Figure 27

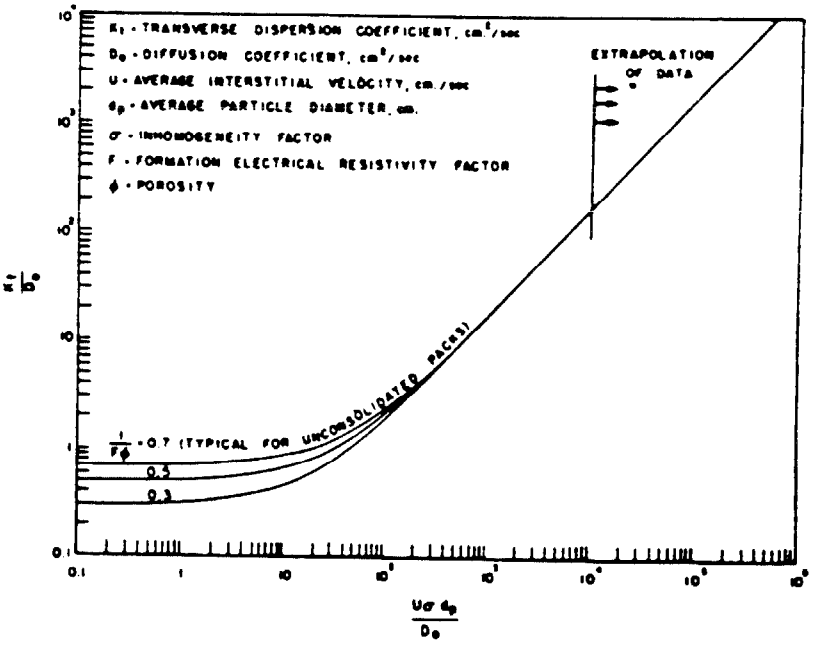


LONGITUDINAL DISPERSION COEFFICIENTS FOR POROUS MEDIA

(after Perkins & Johnston)

SCIENTIFIC SOFTWARE INTERCOMP

Figure 25

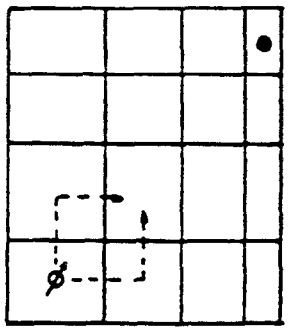


TRANSVERSE DISPERSION COEFFICIENTS FOR POROUS MEDIA

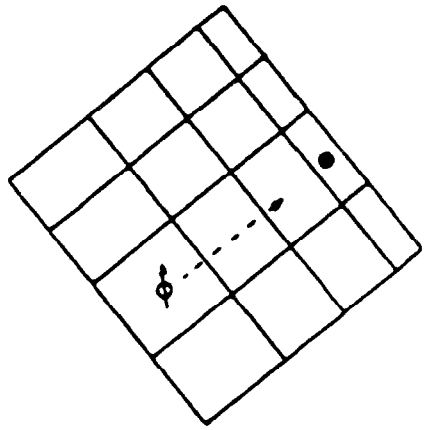
(after Perkins & Johnston)

SCIENTIFIC SOFTWARE INTERCOMP

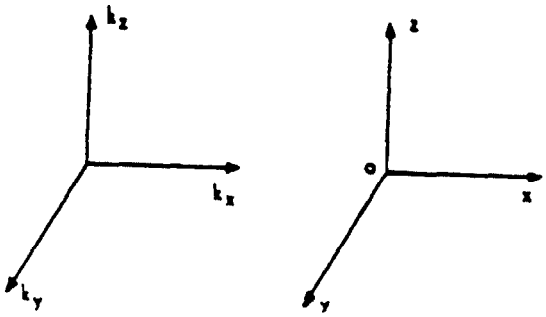
Figure 29



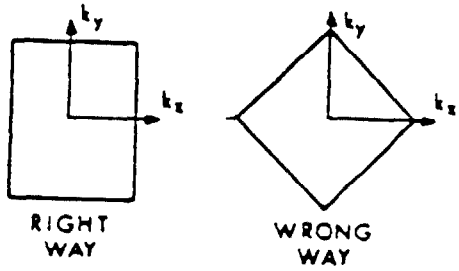
DIAGONAL
GRID



PARALLEL
GRID



3-D ORIENTATION



2-D ORIENTATION

GRID ORIENTATION AND
PRINCIPLE AXES OF
SYMMETRY

SCIENTIFIC SOFTWARE INTERCOMP